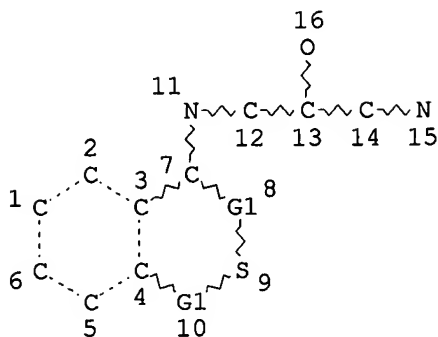


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REP G1=(0-2) C
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC 1
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

=> s l1 ful
 FULL SEARCH INITIATED 07:35:31 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 149 TO ITERATE

100.0% PROCESSED 149 ITERATIONS 95 ANSWERS
 SEARCH TIME: 00.00.01

L3 95 SEA SSS FUL L1

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 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
173.00	173.21

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=> s 13

L4 15 L3

=> d bib abs hitstr 1-15

L4 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:1103733 CAPLUS

DN 143:386930

TI Preparation of 2-amino- and 2-thio-substituted 1,3-diaminopropanes as β -secretase inhibitors for treating Alzheimer's disease and other diseases characterized by deposition of A β -peptide

IN Hom, Roy; Tucker, John; John, Varghese; Shah, Neerav

PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company

SO PCT Int. Appl., 365 pp.

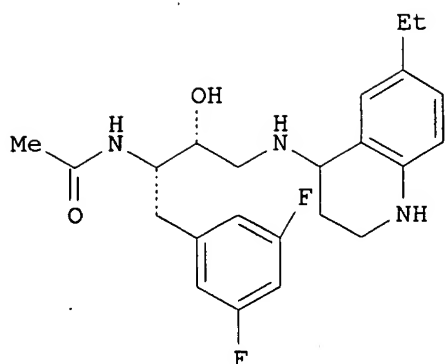
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005095326	A2	20051013	WO 2005-US9920	20050325
	WO 2005095326	A3	20051110		
	WO 2005095326	A8	20061012		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	CA 2560773	A1	20051013	CA 2005-2560773	20050325
	US 2005267199	A1	20051201	US 2005-90520	20050325
	EP 1751091	A2	20070214	EP 2005-741943	20050325
	R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU			
PRAI	US 2004-556461P	P	20040325		
	WO 2005-US9920	W	20050325		
OS	MARPAT 143:386930				
GI					



II

AB Title compds. of formula Z-X-NHCH(R1)CH(Q)C(R2)(R3)N(R15)(Rc) (I) [Q = SH and derivs., NH and derivs.; Z = H, (un)substituted cycloalkylalk(en/yn)yl, cycloalkyl; X = CO, SO₂; R1 = (un)substituted alkyl; R2, R3 = independently H, F, (un)substituted alk(en/yn)yl, hetero/aryl, etc.; R2CR3 = 3-7 membered carbocyclic ring with 1-3 C atoms optionally replaced by O, S, SO₂, CO, NH and derivs.; R15 = H, (un)substituted alkyl, alkoxy, etc.; Rc = (un)substituted (CH₂)_n-cycloalkyl, etc.; n = 0-3] were prepared Compds. disclosed herein are inhibitors of the β -secretase enzyme (no data) and are therefore useful in the treatment of Alzheimer's disease and other diseases characterized by deposition of A beta peptide in a mammal (no data). For example, II was prepared, in 4 steps, by reacting benzyl 4-amino-6-ethyl-3,4-dihydroquinoline-1(2H)-carboxylate with [(1S)-2-(3,5-difluorophenyl)-1-((2S)-oxiran-2-yl)ethyl]carbamate, followed by Boc-deprotection, acetylation in the presence of N,N-diacetyl-O-methylhydroxylamine/CH₂Cl₂, and Cbz-deprotection.

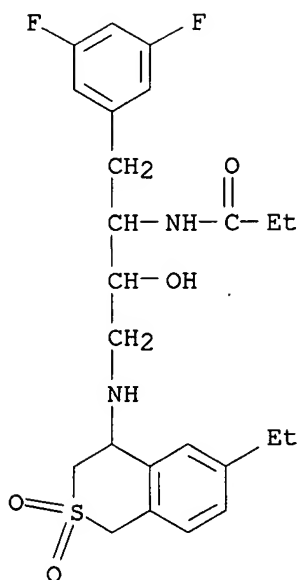
IT 676133-51-0P 676133-52-1P 676133-53-2P
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676133-57-6P 676133-58-7P 676133-59-8P
676133-60-1P 676133-61-2P 676135-54-9P,
N-[(1S,2R)-1-[3-(Allyloxy)-5-fluorobenzyl]-3-[(4R)-6-ethyl-2,2-dioxido-3,4-dihydro-1H-isothiochromen-4-yl)amino]-2-hydroxypropyl]acetamide
676135-56-1P 676135-57-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of 2-amino- and 2-thio-substituted 1,3-diaminopropanes as β -secretase inhibitors for treating Alzheimer's disease and other diseases characterized by deposition of A β -peptide)

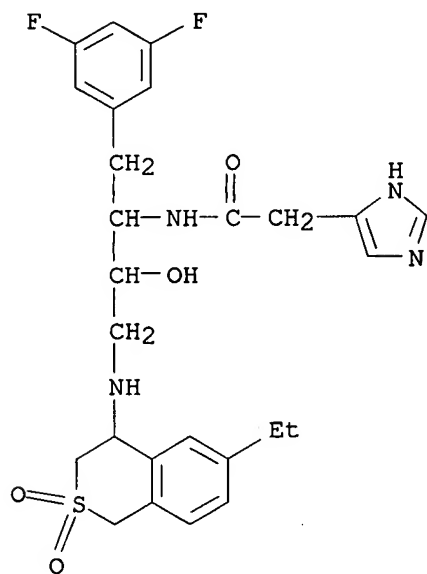
RN 676133-51-0 CAPLUS

CN Propanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)



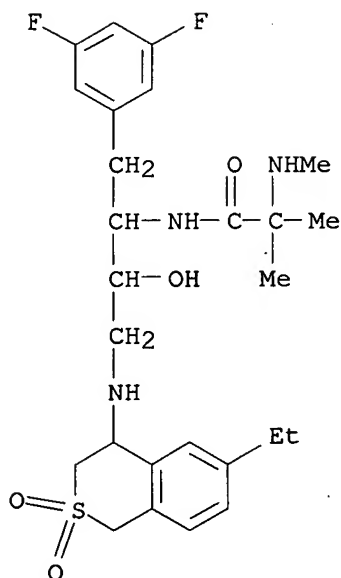
RN 676133-52-1 CAPLUS

CN 1H-Imidazole-4-acetamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-(9CI) (CA INDEX NAME)



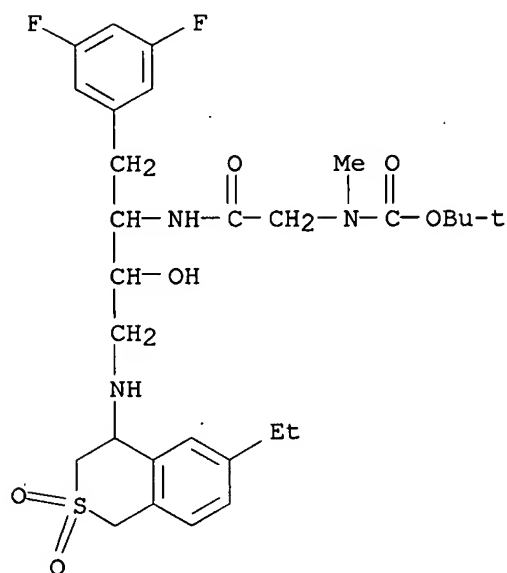
RN 676133-53-2 CAPLUS

CN Propanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-2-methyl-2-(methylamino)- (9CI) (CA INDEX NAME)



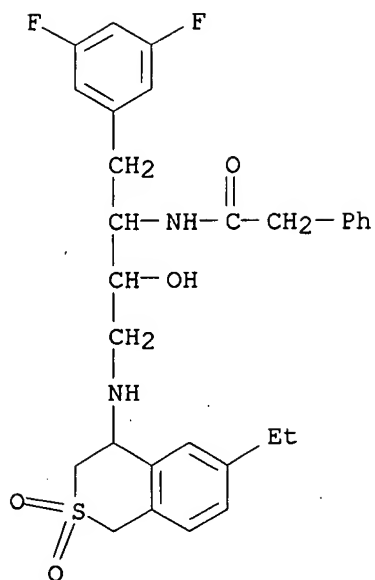
RN 676133-54-3 CAPLUS

CN Carbamic acid, [2-[[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]amino]-2-oxoethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



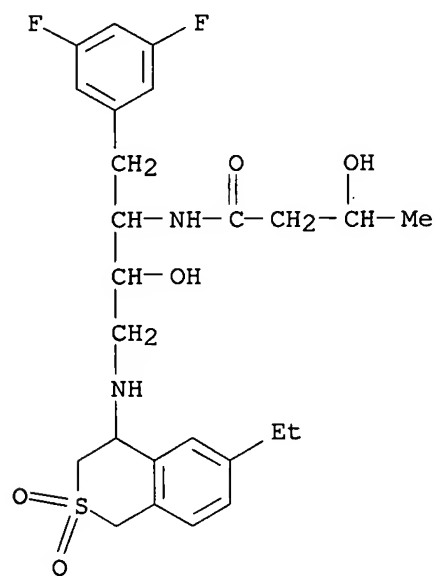
RN 676133-55-4 CAPLUS

CN Benzeneacetamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)



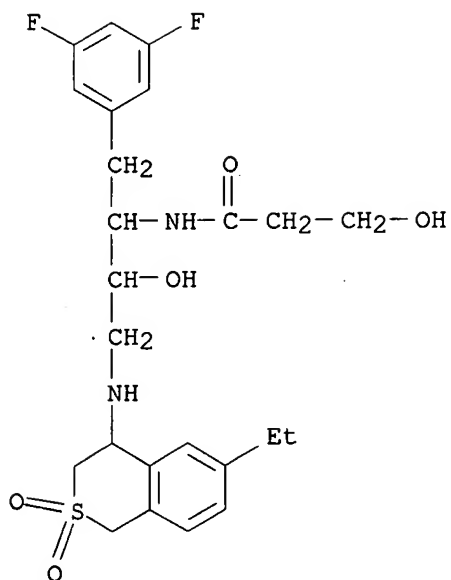
RN 676133-56-5 CAPLUS

CN Butanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3-hydroxy- (9CI)
(CA INDEX NAME)



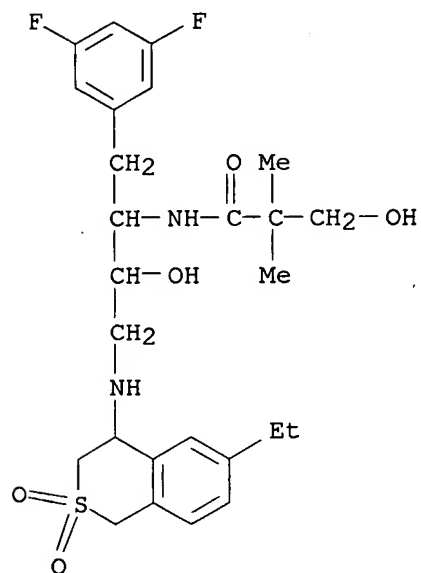
RN 676133-57-6 CAPLUS

CN Propanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3-hydroxy- (9CI)
(CA INDEX NAME)



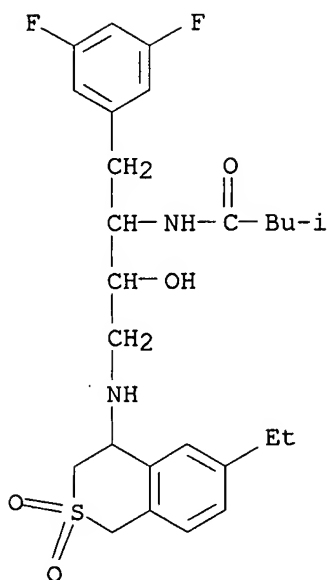
RN 676133-58-7 CAPLUS

CN Propanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3-hydroxy-2,2-dimethyl- (9CI) (CA INDEX NAME)



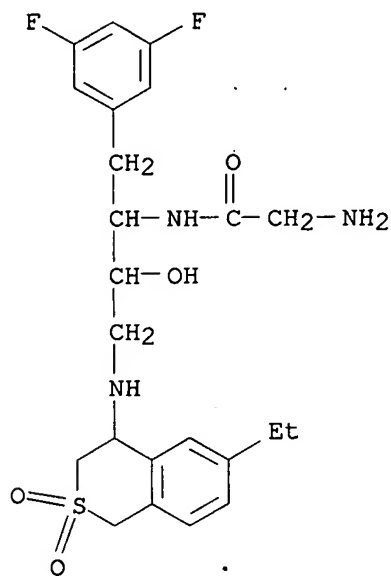
RN 676133-59-8 CAPLUS

CN Butanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3-methyl- (9CI) (CA INDEX NAME)



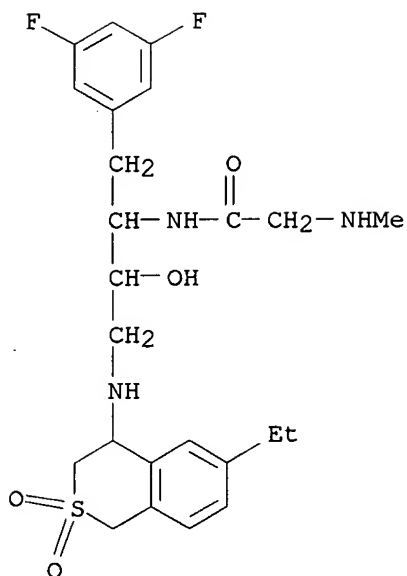
RN 676133-60-1 CAPLUS

CN Acetamide, 2-amino-N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-2-hydroxypropyl]-(9CI) (CA INDEX NAME)



RN 676133-61-2 CAPLUS

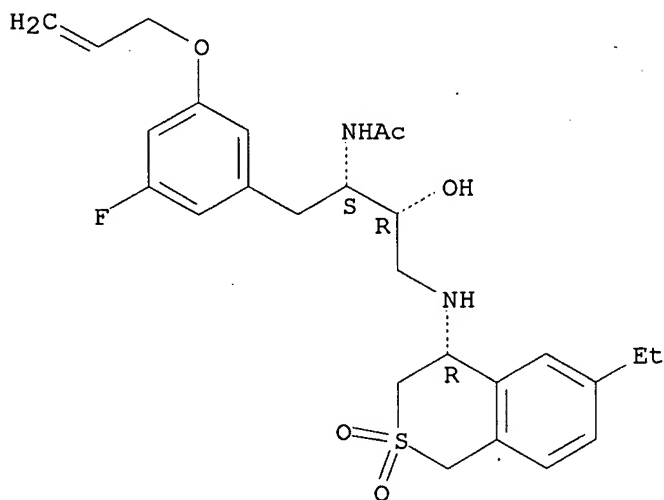
CN Acetamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-2-(methylamino)-(9CI) (CA INDEX NAME)



RN 676135-54-9 CAPLUS

CN Acetamide, N-[(1S,2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-1-[[3-fluoro-5-(2-propenyloxy)phenyl]methyl]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

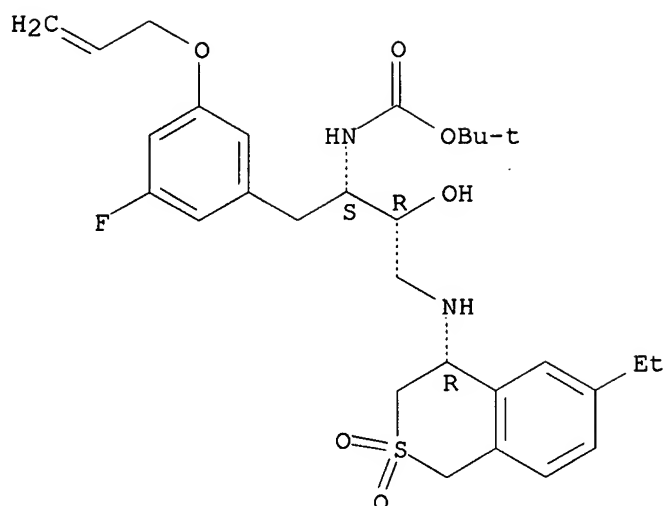
Absolute stereochemistry.



RN 676135-56-1 CAPLUS

CN Carbamic acid, [(1S,2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-1-[[3-fluoro-5-(2-propenyloxy)phenyl]methyl]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

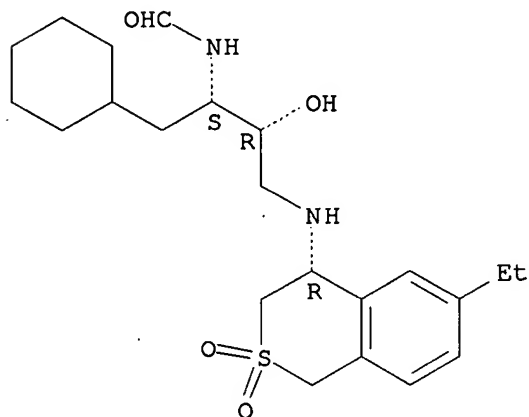
Absolute stereochemistry.



RN 676135-57-2 CAPLUS

CN Formamide, N-[(1S,2R)-1-(cyclohexylmethyl)-3-[[4-(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:1026925 CAPLUS

DN 143:326226

TI Preparation of bicyclic compounds as aspartyl protease and β secretase inhibitors for treating conditions associated with amyloidosis such as Alzheimer's disease

IN John, Varghese; Maillard, Michel; Fang, Lawrence; Tucker, John; Brogley, Louis; Aquino, Jose; Bowers, Simeon; Probst, Gary; Tung, Jay

PA Elan Pharmaceuticals, Inc., USA

SO PCT Int. Appl., 428 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005087714	A2	20050922	WO 2005-US7774	20050309

WO 2005087714 A3 20051215

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

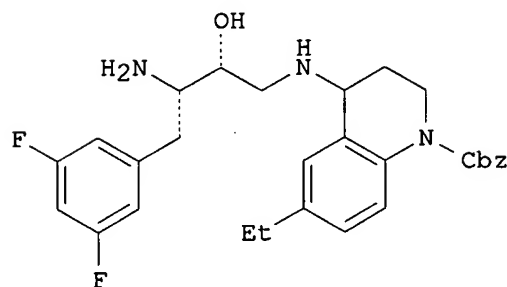
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CA 2556826 A1 20050922 CA 2005-2556826 20050309
 US 2005239832 A1 20051027 US 2005-74828 20050309
 EP 1734961 A2 20061227 EP 2005-725122 20050309

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR

PRAI US 2004-551050P P 20040309
 US 2004-551051P P 20040309
 US 2004-575828P P 20040602
 US 2004-576008P P 20040602
 US 2004-591926P P 20040729
 US 2004-591966P P 20040729
 US 2004-614034P P 20040930
 US 2004-614059P P 20040930
 WO 2005-US7774 W 20050309

OS MARPAT 143:326226
 GI



I

AB The invention relates to compds. of formula $R_2CH_2C(O)NHCHR_1CH(OH)CH_2NHR_c$ (I); [R₁ = (un)substituted benzyl, thien-2-ylmethyl, piperidin-2-ylmethyl, etc.; R₂ = COCH₃, aryl-CO, SO₂-aryl, etc.; R_c = quinolin-4-yl, tetrahydronaphthalen-1-yl, thiochromen-4-yl, etc.; with addnl. details are given in the claims], e.g. (1S,2R)-II, that are useful in treating diseases, disorders, and conditions associated with amyloidosis. Amyloidosis refers to a collection of diseases, disorders, and conditions associated with abnormal deposition of A- β protein. For example, (1S,2R)-II was prepared via ring opening of tert-Bu [(1S)-2-(3,5-difluorophenyl)-1-((2S)-oxiranyl)ethyl]carbamate with benzyl 4-amino-6-ethyl-3,4-dihydroquinoline-1(2H)-carboxylate. Efficacy for 5 examples of I for inhibiting amyloid- β peptide in the cortex and/or plasma are tabulated. The selectivity of I for β -secretase vs. cathepsin D for 2 examples of I are tabulated. Oral bioavailability for four I was determined in male rats. Brain uptake, total polar surface area and/or lipophilicity for 5 examples of I are tabulated.

IT 676135-54-9P, N-[(1S,2R)-1-[3-(Allyloxy)-5-fluorobenzyl]-3-[(4R)-6-ethyl-2,2-dioxido-3,4-dihydro-1H-isothiochromen-4-yl)amino]-2-hydroxypropyl]acetamide 865472-26-0P, N-[(1S,2R)-1-

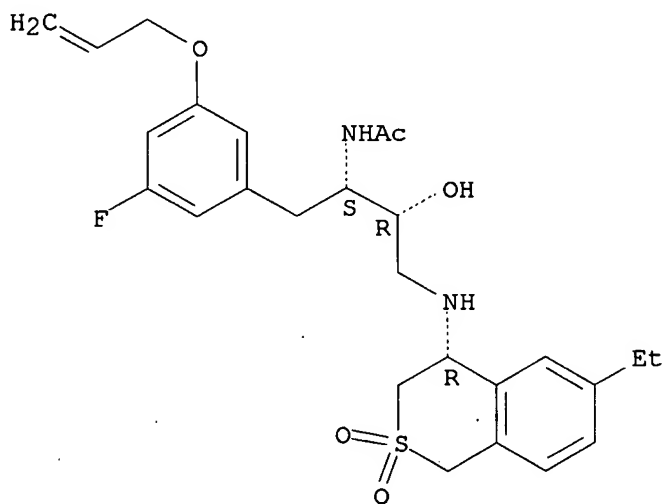
(Cyclohexylmethyl)-3-[[[(4R)-6-ethyl-2,2-dioxido-3,4-dihydro-1H-isothiochroman-4-yl]amino]-2-hydroxypropyl]acetamide 865472-45-3P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of bicyclic compds. as aspartyl protease and β secretase inhibitors for treating conditions associated with amyloidosis such as Alzheimer's disease)

RN 676135-54-9 CAPLUS

CN Acetamide, N-[(1S,2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-1-[[3-fluoro-5-(2-propenyloxy)phenyl]methyl]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

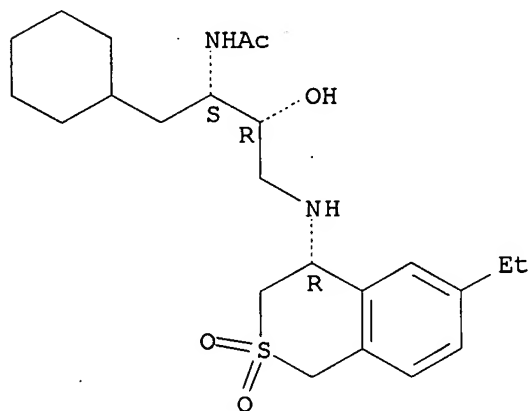
Absolute stereochemistry.



RN 865472-26-0 CAPLUS

CN Acetamide, N-[(1S,2R)-1-(cyclohexylmethyl)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

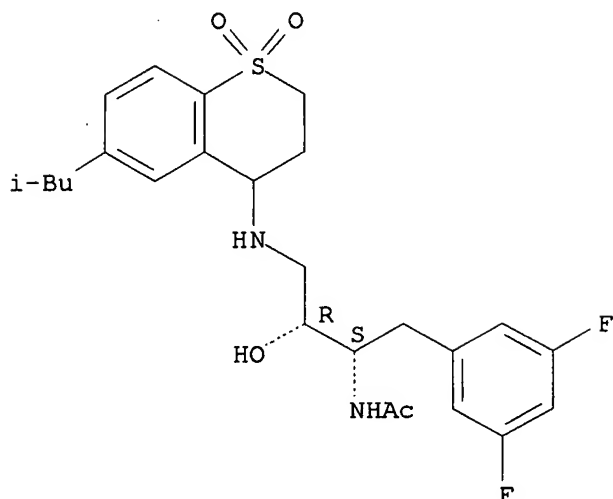
Absolute stereochemistry.



RN 865472-45-3 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[3,4-dihydro-6-(2-methylpropyl)-1,1-dioxido-2H-1-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 865472-41-9P 865472-42-0P 865472-43-1P
865472-44-2P

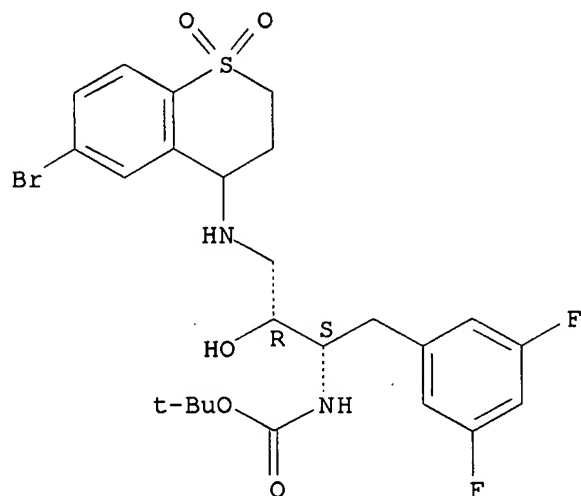
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of bicyclic compds. as aspartyl protease and β secretase inhibitors for treating conditions associated with amyloidosis such as Alzheimer's disease)

RN 865472-41-9 CAPLUS

CN Carbamic acid, [(1S,2R)-3-[(6-bromo-3,4-dihydro-1,1-dioxido-2H-1-benzothiopyran-4-yl)amino]-1-[(3,5-difluorophenyl)methyl]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

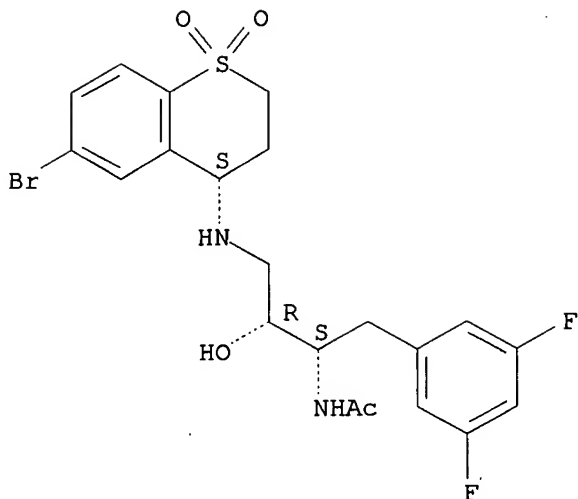
Absolute stereochemistry.



RN 865472-42-0 CAPLUS

CN Acetamide, N-[(1S,2R)-3-[[[(4S)-6-bromo-3,4-dihydro-1,1-dioxido-2H-1-benzothiopyran-4-yl]amino]-1-[(3,5-difluorophenyl)methyl]-2-hydroxypropyl]]- (9CI) (CA INDEX NAME)

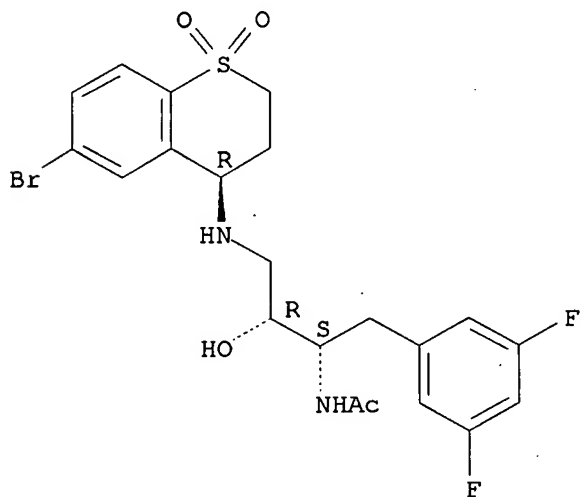
Absolute stereochemistry.



RN 865472-43-1 CAPLUS

CN Acetamide, N-[(1S,2R)-3-[[(4R)-6-bromo-3,4-dihydro-1,1-dioxido-2H-1-benzothiopyran-4-yl]amino]-1-[(3,5-difluorophenyl)methyl]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

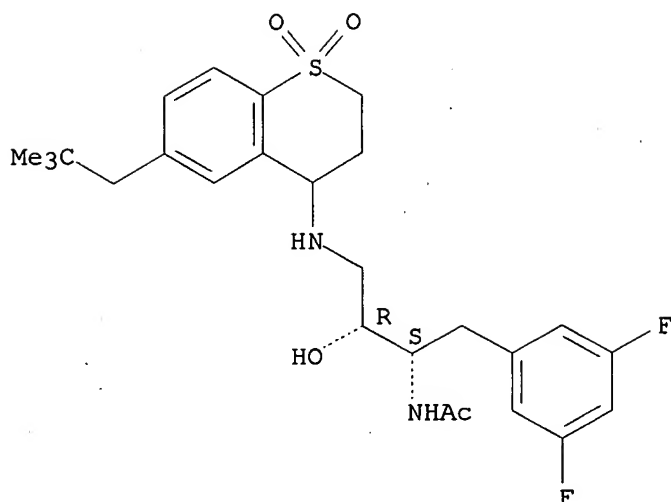
Absolute stereochemistry.



RN 865472-44-2 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[6-(2,2-dimethylpropyl)-3,4-dihydro-1,1-dioxido-2H-1-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:1021743 CAPLUS

DN 143:326360

TI Preparation of hydroxyethylamines as aspartyl protease inhibitors for treatment of amyloidosis.

IN John, Varghese; Maillard, Michel; Tucker, John; Aquino, Jose; Jagodzinska, Barbara; Brogley, Louis; Tung, Jay; Bowers, Simeon; Dressen, Darren; Probst, Gary; Shah, Neerav

PA Elan Pharmaceuticals, Inc., USA

SO PCT Int. Appl., 403 pp.

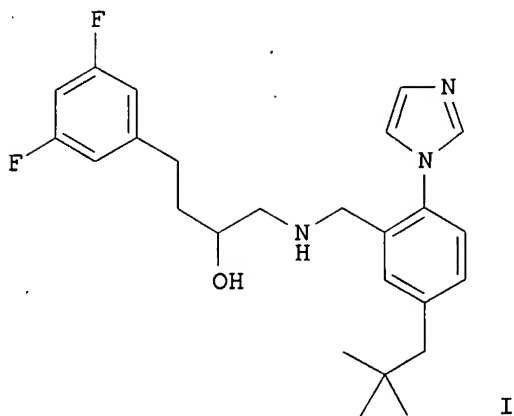
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005087751	A2	20050922	WO 2005-US7771	20050309
	WO 2005087751	A3	20051215		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	CA 2558034	A1	20050922	CA 2005-2558034	20050309
	US 2005239836	A1	20051027	US 2005-75312	20050309
	EP 1730125	A2	20061213	EP 2005-725119	20050309
	R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR			
PRAI	US 2004-551052P	P	20040309		
	US 2004-575977P	P	20040602		
	US 2004-591918P	P	20040729		
	US 2004-619918P	P	20041020		
	WO 2005-US7771	W	20050309		
OS	MARPAT 143:326360				
GI					



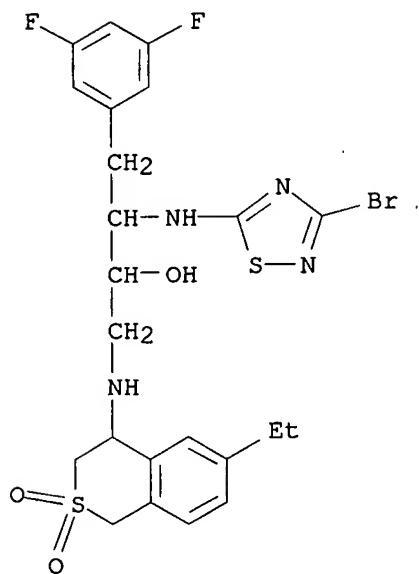
AB R1R2CHCH(OH)CH2NHRc [R1 = (substituted) QL; Q = (substituted) Ph, thienyl, (hetero)cycloalkyl; L = O, SO2, CO, CR55R60, CH(NR55R60); R55, R60 = H, alkyl; R2 = H, OH, (substituted) alkoxy, aryloxy, alkyl, alkylamino, heterocycloalkyl, heterocycloalkylamino, (substituted) amino, aminocarbonyl, etc.; Rc = (substituted) cycloalkyl(alkyl), alkyl, etc.; with provisos], were prepared. Thus, title compound (I) inhibited β -secretase with $IC_{50} = 1.1 \mu M$.

IT 865177-47-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of hydroxyethylamines as aspartyl protease inhibitors for treatment of amyloidosis)

RN 865177-47-5 CAPLUS

CN Benzenepropanol, β -[(3-bromo-1,2,4-thiadiazol-5-yl)amino]- α -[[[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]methyl]-3,5-difluoro- (9CI) (CA INDEX NAME)



IT 865177-66-8P

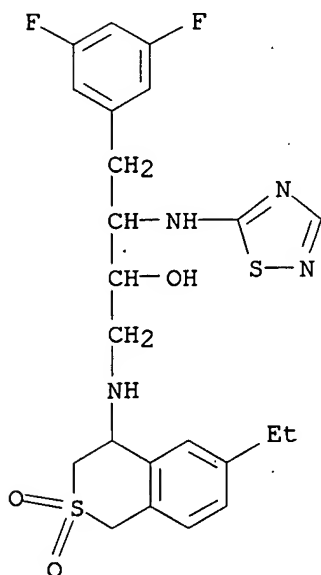
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(preparation of hydroxyethylamines as aspartyl protease inhibitors for treatment of amyloidosis)

RN 865177-66-8 CAPLUS

CN Benzenepropanol, α -[[[6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]methyl]-3,5-difluoro- β -(1,2,4-thiadiazol-5-ylamino)- (9CI) (CA INDEX NAME)



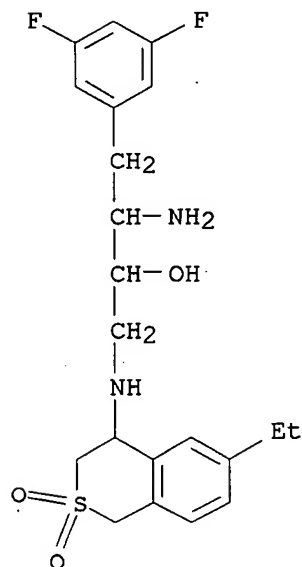
IT 865178-47-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of hydroxyethylamines as aspartyl protease inhibitors for treatment of amyloidosis)

RN 865178-47-8 CAPLUS

CN Benzenepropanol, β -amino- α -[[[6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]methyl]-3,5-difluoro- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:1021606 CAPLUS

DN 143:326096

TI Preparation of substituted urea and carbamate, phenacyl-2-hydroxy-3-diaminoalkane, and benzamide-2-hydroxy-3-diaminoalkane aspartyl protease and β -secretase inhibitors for treating conditions associated with amyloidosis such as Alzheimer's disease

IN John, Varghese; Maillard, Michel; Tucker, John; Aquino, Jose; Hom, Roy; Tung, Jay; Dressen, Darren; Shah, Neerav; Neitz, R. Jeffrey

PA Elan Pharmaceuticals, Inc., USA

SO PCT Int. Appl., 532 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005087215	A1	20050922	WO 2005-US7775	20050309
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	RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	CA 2558249	A1	20050922	CA 2005-2558249	20050309
	US 2005261273	A1	20051124	US 2005-75292	20050309
	EP 1734942	A1	20061227	EP 2005-725123	20050309
	R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR			
PRAI	US 2004-551192P	P	20040309		
	US 2004-575829P	P	20040602		
	US 2004-591857P	P	20040729		
	US 2004-622589P	P	20041028		
	WO 2005-US7775	W	20050309		

OS MARPAT 143:326096

AB The invention is related to compds. of formula $R_2NHCH(R_1)CH(OH)CH_2NHR_c$ (I) [R₁ = (un)substituted benzyl, thien-2-ylmethyl, etc.; R₂ = NH₂ and derivs., SO₂-aryl, hetero/aryl-U, etc.; U = CO, CS, CONH and derivs., etc.; R_c = carbocyclyl or heterocyclyl; with addnl. details given in the claims] particularly acetyl 2-hydroxy-1,3-diaminospirocyclohexanes and derivs., that are useful in treating diseases, disorders, and conditions associated with amyloidosis. Amyloidosis refers to a collection of diseases, disorders, and conditions associated with abnormal deposition of A- β protein. For example, alkylation of (2R,3S)-3-amino-1-[[1-(3-tert-butylphenyl)cyclohexyl]amino]-4-(3,5-difluorophenyl)butan-2-ol \cdot 2HCl with 4-iodobenzamide gave the corresponding amide. Selected I displayed IC₅₀ values < 5 μ M in a cell free inhibition assay utilizing a synthetic APP substrate that can be cleaved by β -secretase. The selectivity of I for β -secretase vs. cathepsin D for 6 examples of I are tabulated. Brain uptake, total polar surface area and/or lipophilicity for 32 examples of I are tabulated.

IT 676135-54-9P, N-[(1S,2R)-1-[3-(Allyloxy)-5-fluorobenzyl]-3-[[[(4R)-6-ethyl-2,2-dioxido-3,4-dihydro-1H-isothiochromen-4-yl]amino]-2-hydroxypropyl]acetamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

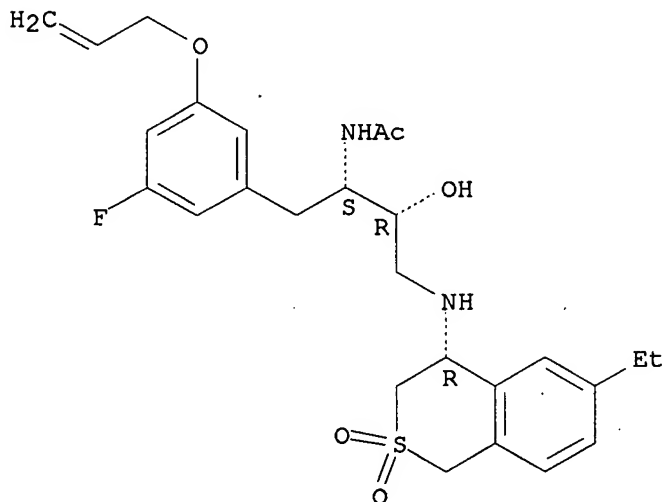
(Uses)

(drug candidate; preparation of as aspartyl protease and β -secretase inhibitors)

RN 676135-54-9 CAPLUS

CN Acetamide, N-[(1S,2R)-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-1-[[3-fluoro-5-(2-propenyloxy)phenyl]methyl]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:696731 CAPLUS

DN 143:193724

TI Preparation of N-(3-amino-2-hydroxypropyl)acetamides as aspartyl protease and beta secretase inhibitors for treating conditions associated with amyloidosis such as Alzheimer's disease

IN John, Varghese; Hom, Roy; Sealy, Jennifer; Aquino, Jose; Probst, Gary; Tung, Jay; Fang, Larry

PA Elan Pharmaceuticals, Inc., USA

SO PCT Int. Appl., 499 pp.

CODEN: PIXXD2

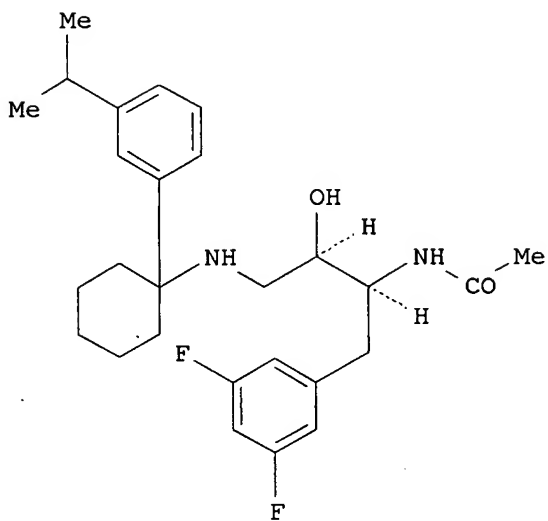
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005070407	A1	20050804	WO 2005-US1875	20050121
	W:				
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	RW:				
	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2553973	A1	20050804	CA 2005-2553973	20050121

US 2006014790	A1	20060119	US 2005-38790	20050121
EP 1729755	A1	20061213	EP 2005-711743	20050121
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,				
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRAI	US 2004-537522P	P	20040121	
	US 2004-537551P	P	20040121	
	US 2004-537580P	P	20040121	
	US 2004-575798P	P	20040602	
	US 2004-575799P	P	20040602	
	US 2004-575858P	P	20040602	
	US 2004-591858P	P	20040729	
	US 2004-591885P	P	20040729	
	US 2004-591908P	P	20040729	
	US 2004-619917P	P	20041020	
	US 2004-619947P	P	20041020	
	US 2004-619948P	P	20041020	
	WO 2005-US1875	W	20050121	
OS	MARPAT 143:193724			
GI				



AB The invention relates to N-(3-amino-2-hydroxypropyl)acetamides (R₂CH₂C(O)NHCHR₁CH(OH)CH₂NHR_c (I); R₁ = (un)substituted benzyl, thien-2-ylmethyl, etc.; R₂ = H and F; R_c = carbocyclyl or heterocyclyl; addnl. details are given in the claims; e.g. N-[(1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-3-[[1-(3-isopropylphenyl)cyclohexyl]amino]propyl]acetamide hydrochloride (free base shown as II)) that are useful in treating diseases, disorders, and conditions associated with amyloidosis. Amyloidosis refers to a collection of diseases, disorders, and conditions associated with abnormal deposition of A-beta protein. Although the methods of preparation are not claimed, .apprx.200 example preps. of I and intermediates are included. For example, II was prepared in 3 steps (77, unknown and 87% yields) starting from 1-(3-isopropylphenyl)cyclohexanamine hydrochloride and [(1S)-2-(3,5-difluorophenyl)-1-((2S)-oxiran-2-yl)ethyl]carbamic acid tert-Bu ester and involving intermediates tert-Bu [(1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-3-[[1-(3-isopropylphenyl)cyclohexyl]amino]propyl]carbamate and (2R,3S)-3-amino-4-(3,5-difluorophenyl)-1-[[1-(3-isopropylphenyl)cyclohexyl]amino]butan-2-ol dihydrochloride. Efficacy for 10 examples of I for inhibiting

amyloid-beta peptide in the cortex and/or plasma are tabulated. The selectivity of I for β -secretase vs. cathepsin D for 92 examples of I are tabulated. Oral bioavailability for one I was determined in male rats. Brain uptake, total polar surface area and/or lipophilicity for 32 examples of I are tabulated.

IT 676135-54-9P, N-[(1S,2R)-1-[3-(Allyloxy)-5-fluorobenzyl]-3-[(4R)-6-ethyl-2,2-dioxido-3,4-dihydro-1H-isothiochromen-4-yl]amino]-2-hydroxypropyl]acetamide

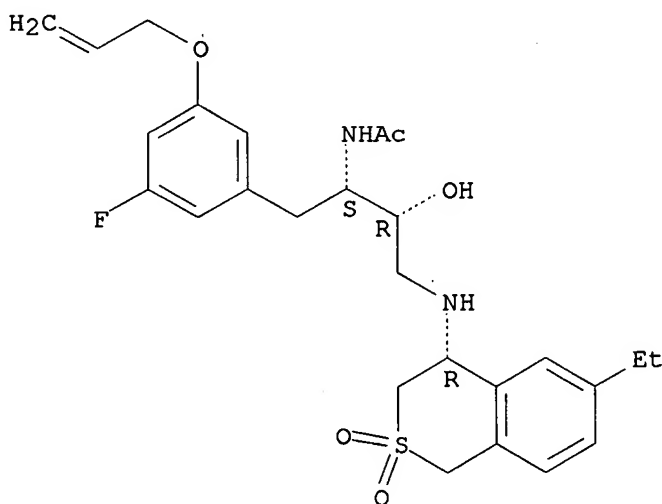
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of N-(3-amino-2-hydroxypropyl)acetamides as aspartyl protease and beta secretase inhibitors for treating conditions associated with amyloidosis such as Alzheimer's disease)

RN 676135-54-9 CAPLUS

CN Acetamide, N-[(1S,2R)-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-1-[3-fluoro-5-(2-propenyloxy)phenyl]methyl]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:927201 CAPLUS

DN 141:395188

TI Preparation of phenacyl-substituted 2-hydroxy-3-diaminoalkanes as inhibitors of β -secretase

IN Aquino, Jose; John, Varghese; Tucker, John A.; Hom, Roy; Pulley, Shon; Tenbrink, Ruth

PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company

SO PCT Int. Appl., 106 pp.

CODEN: PIXXD2

DT Patent

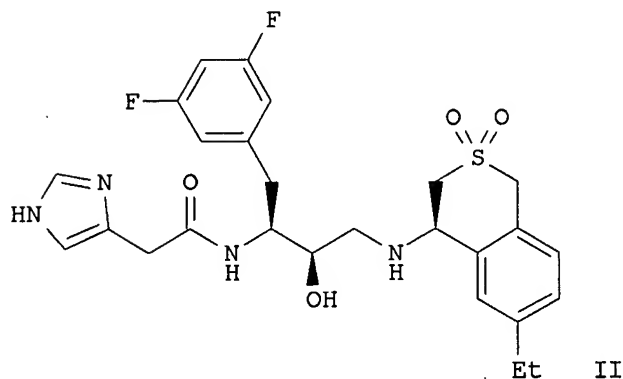
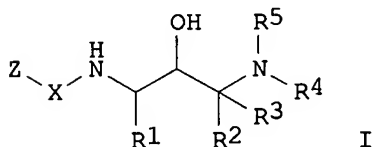
LA English

FAN.CNT 1

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GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW,
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
 SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
 TD, TG

CA 2522805 A1 20041104 CA 2004-2522805 20040421
 US 2005054690 A1 20050310 US 2004-828582 20040421
 EP 1615915 A1 20060118 EP 2004-760106 20040421
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
 BR 2004009627 A 20060425 BR 2004-9627 20040421
 JP 2006524258 T 20061026 JP 2006-513208 20040421
 PRAI US 2003-464676P P 20030421
 WO 2004-US12384 W 20040421
 OS CASREACT 141:395188; MARPAT 141:395188
 GI



AB Title compds. I [Z = divalent (un)substituted alkyl; X = CO, SO₂; R₁ = alkyl; R₂-3 = H, F, alkyl, etc.; R₄ = alkyl, cycloalkyl, etc.; R₅ = H, alkyl, alkoxy, etc.] are prepared For instance, the preparation of II from (R)-7-bromo-1,2,3,4-tetrahydro-1-naphthylamine•HCl (preparation given) is described in general procedures. I are inhibitors of β-secretase and useful for the treatment of Alzheimer's disease and other similar diseases and other diseases characterized by deposition of Aβ peptide.

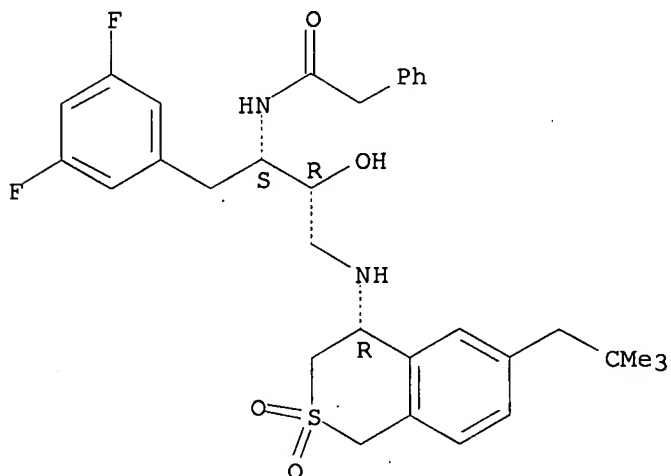
IT 785829-29-0P 785829-31-4P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (claimed compound; preparation of phenacyl-substituted 2-hydroxy-3-

diaminoalkanes as inhibitors of β -secretase)

RN 785829-29-0 CAPLUS

CN Benzeneacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-(2,2-dimethylpropyl)-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

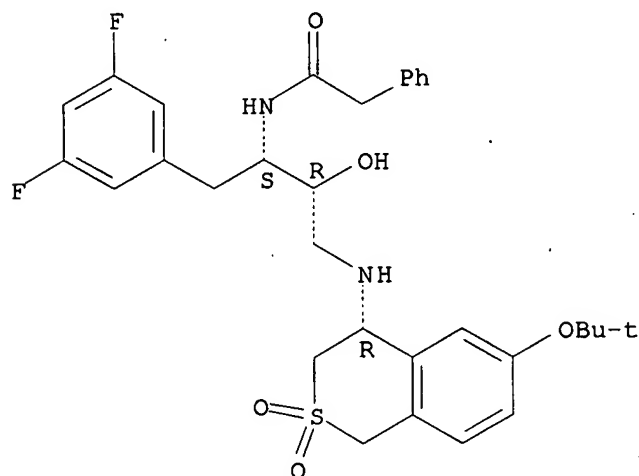
Absolute stereochemistry.



RN 785829-31-4 CAPLUS

CN Benzeneacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-(1,1-dimethylethoxy)-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 527732-56-5P 527732-60-1P 527733-13-7P

785828-93-5P 785828-95-7P 785828-97-9P

785828-99-1P 785829-01-8P 785829-03-0P

785829-05-2P 785829-07-4P 785829-09-6P

785829-11-0P 785829-13-2P 785829-15-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

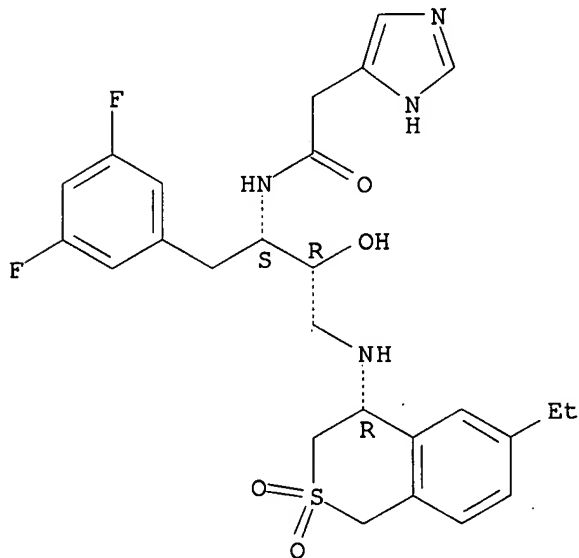
(preparation of phenacyl-substituted 2-hydroxy-3-diaminoalkanes as

inhibitors of β -secretase)

RN 527732-56-5 CAPLUS

CN 1H-Imidazole-4-acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

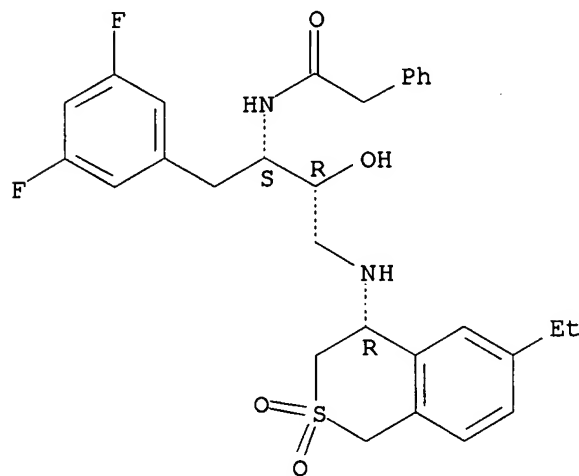
Absolute stereochemistry.



RN 527732-60-1 CAPLUS

CN Benzeneacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

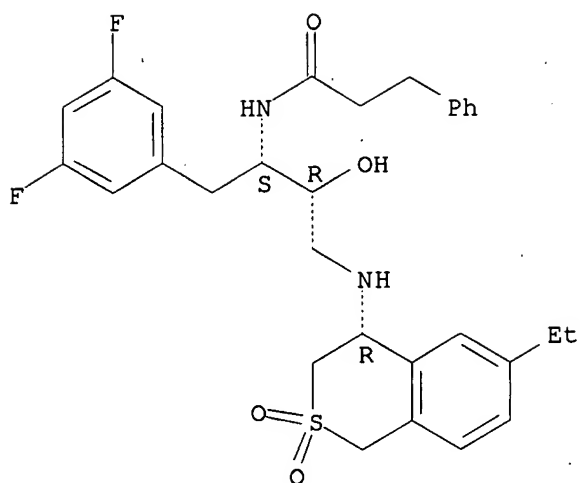
Absolute stereochemistry.



RN 527733-13-7 CAPLUS

CN Benzenepropanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

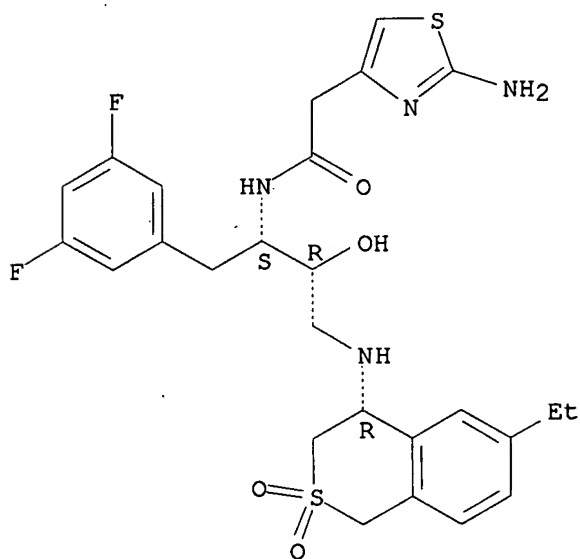
Absolute stereochemistry.



RN 785828-93-5 CAPLUS

CN 4-Thiazoleacetamide, 2-amino-N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

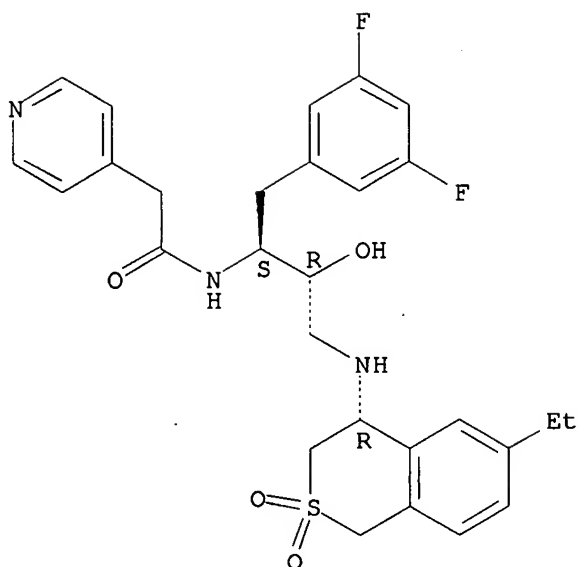
Absolute stereochemistry.



RN 785828-95-7 CAPLUS

CN 4-Pyridineacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

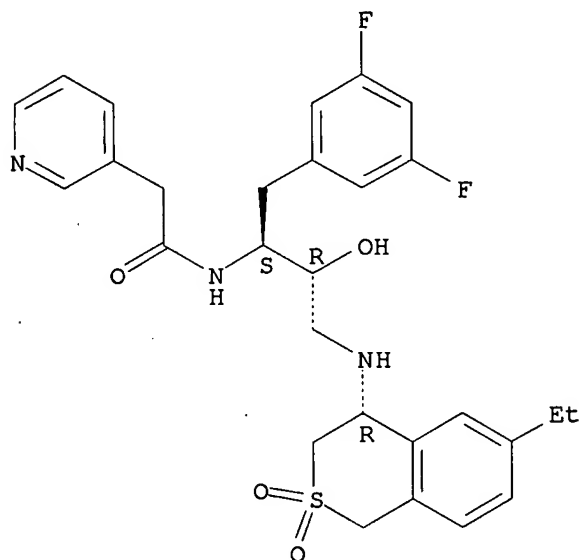
Absolute stereochemistry.



RN 785828-97-9 CAPLUS

CN 3-Pyridineacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

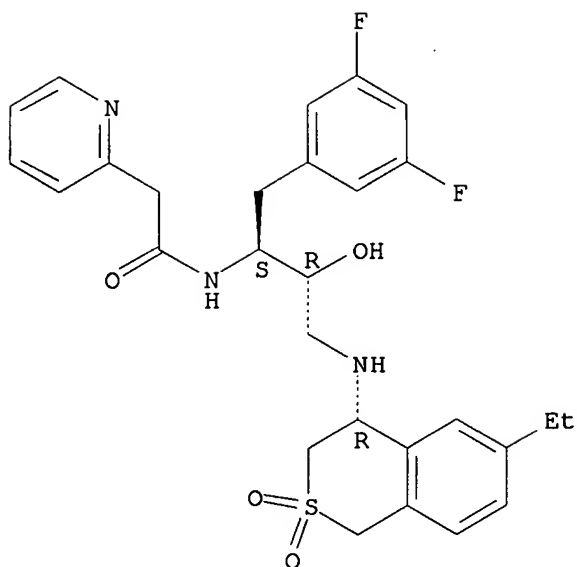
Absolute stereochemistry.



RN 785828-99-1 CAPLUS

CN 2-Pyridineacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

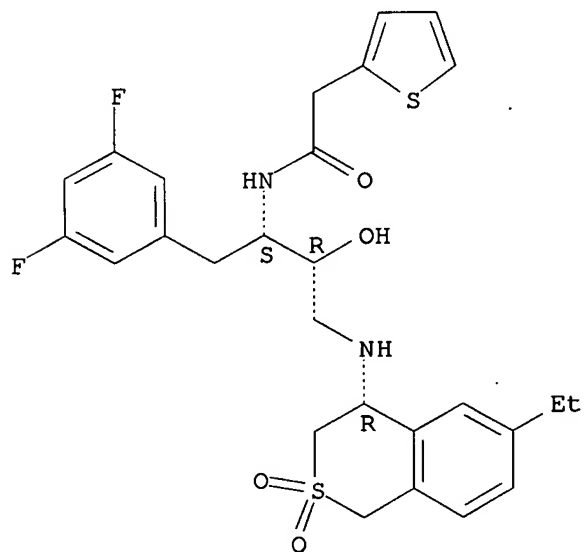
Absolute stereochemistry.



RN 785829-01-8 CAPLUS

CN 2-Thiopheneacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

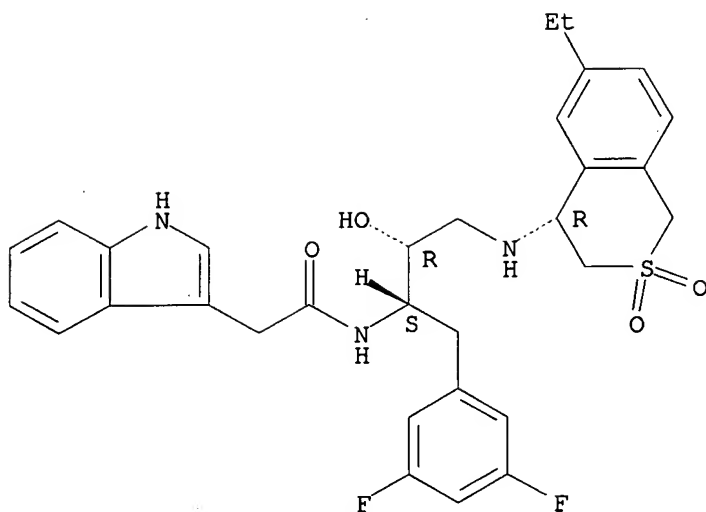
Absolute stereochemistry.



RN 785829-03-0 CAPLUS

CN 1H-Indole-3-acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

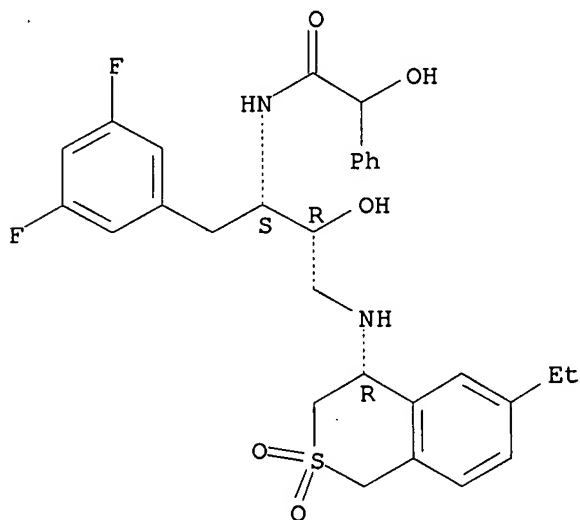
Absolute stereochemistry.



RN 785829-05-2 CAPLUS

CN Benzeneacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-α-hydroxy- (9CI) (CA INDEX NAME)

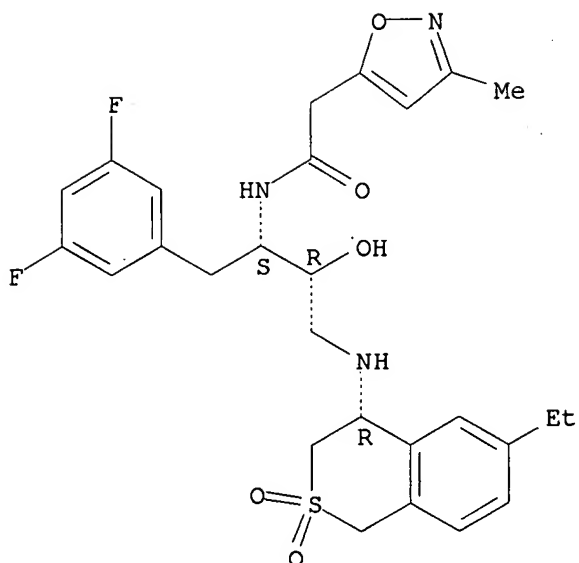
Absolute stereochemistry.



RN 785829-07-4 CAPLUS

CN 5-Isoxazoleacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-methyl- (9CI) (CA INDEX NAME)

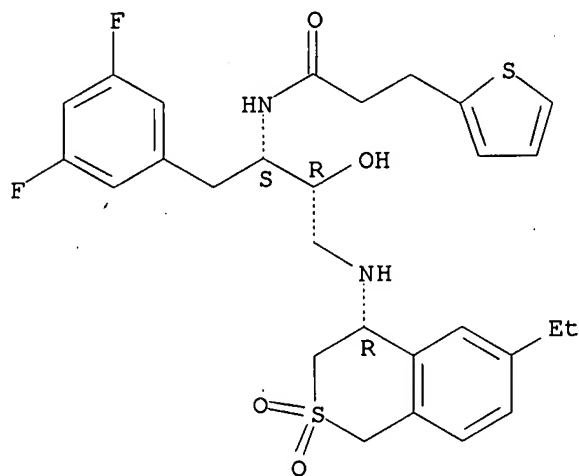
Absolute stereochemistry.



RN 785829-09-6 CAPLUS

CN 2-Thiophenepropanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

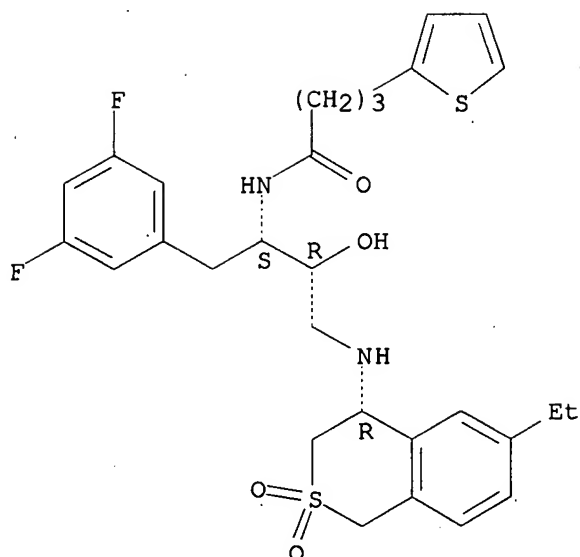
Absolute stereochemistry.



RN 785829-11-0 CAPLUS

CN 2-Thiophenebutanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

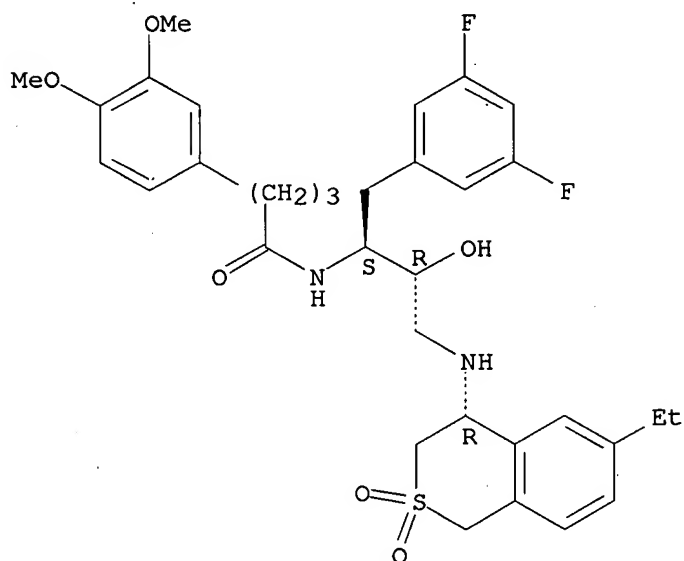
Absolute stereochemistry.



RN 785829-13-2 CAPLUS

CN Benzenebutanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3,4-dimethoxy- (9CI) (CA INDEX NAME)

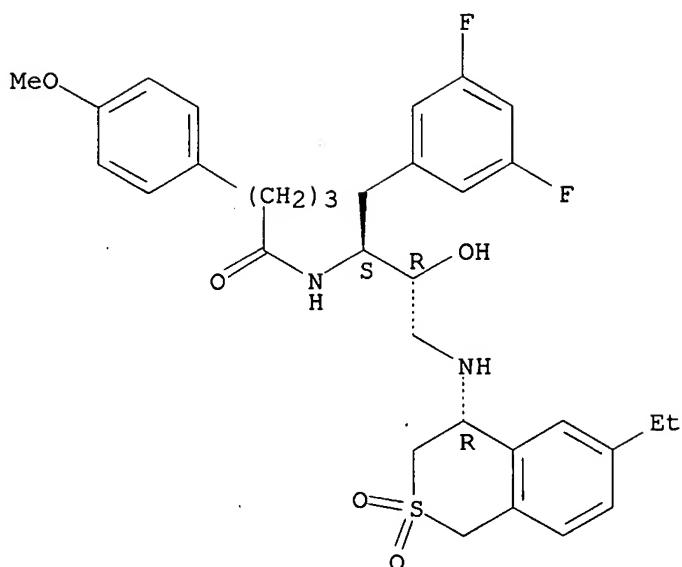
Absolute stereochemistry.



RN 785829-15-4 CAPLUS

CN Benzenebutanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-4-methoxy- (9CI) (CA INDEX NAME)

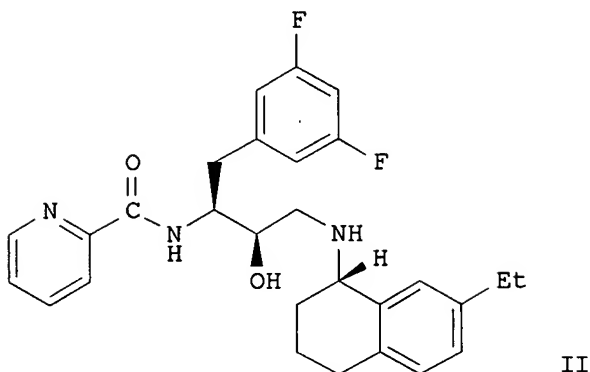
Absolute stereochemistry.



RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:927177 CAPLUS
DN 141:395294
TI Preparation of 2-hydroxy-3-aminoalkylbenzamides as β -secretase
inhibitors for the treatment of Alzheimer's disease
IN Aquino, Jose; John, Varghese; Tucker, John A.; Hom, Roy; Pulley, Shon;
Tenbrink, Ruth
PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SO PCT Int. Appl., 101 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004094384	A2	20041104	WO 2004-US12197	20040421
	WO 2004094384	A3	20050203		
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	CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,				
	GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,				
	LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,				
	NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,				
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	RW:				
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	ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,				
	SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,				
	TD, TG				
	CA 2523232	A1	20041104	CA 2004-2523232	20040421
	US 2005032848	A1	20050210	US 2004-829106	20040421
	US 7223774	B2	20070529		
	EP 1615892	A2	20060118	EP 2004-760050	20040421
	R:				
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	IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
	BR 2004009624	A	20060418	BR 2004-9624	20040421
	JP 2006524255	T	20061026	JP 2006-513163	20040421
PRAI	US 2003-464687P	P	20030421		



AB The present invention relates to 2-hydroxy-3-aminoalkylbenzamides, Z-X-NH-C(R1)-C(OH)-C(R2R3)-NR15Rc [I; Z = (un)substituted hetero/aryl, heterocyclyl; X = CO, SO₂; R1 = (un)substituted alkyl; R2, R3 = independently H, F, (un)substituted alk(en/yn)yl, cycloalkyl; or R2CR3 = C3-C7-carbocycle, wherein one carbon is optionally replaced by O, S, SO₂, etc.; R15 = H, (un)substituted alkoxy/hydroxy/halo/alkyl, alkoxy; Rc = (un)substituted (CH₂)₀₋₃-cycloalkyl, monocyclic or bicyclic ring, alkenyl, etc.] useful in treating Alzheimer's disease and similar diseases. These compds. include inhibitors of the beta-secretase enzyme (no data) that are useful in the treatment of Alzheimer's disease and other diseases characterized by deposition of A beta peptide in a mammal. The compds. of the invention are useful in pharmaceutical compns. and methods of treatment to reduce A beta peptide formation. 8 Synthetic examples of intermediates, characterization data for 11 examples, e.g. II, and another 18 claimed examples of I are included. General procedures for the preparation of compds. I are given. I displayed IC₅₀ values < 50 μM in a β-secretase inhibition assay. Selected I exhibited IC₅₀ < 5 μM in a cell free β-secretase inhibition assay.

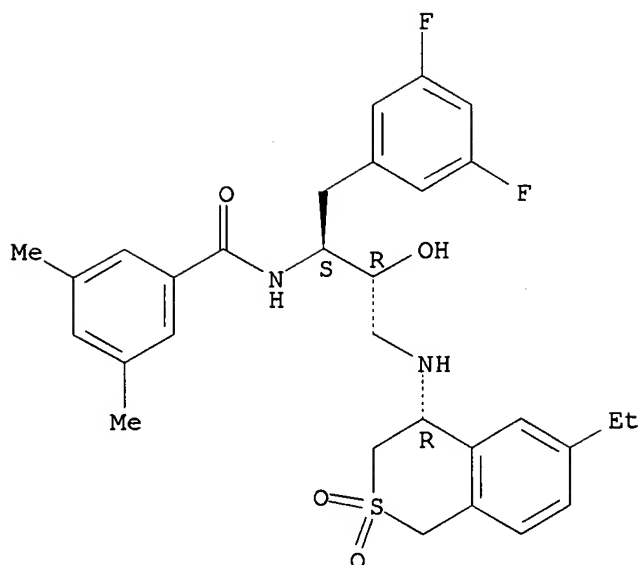
IT 527731-85-7P, N-[(1S,2R)-1-(3,5-Difluorobenzyl)-3-[(4R)-6-ethyl-2,2-dioxido-3,4-dihydro-1H-isothiochromen-4-yl)amino]-2-hydroxypropyl]-3,5-dimethylbenzamide 527733-19-3P, N-[(1S,2R)-1-(3,5-Difluorobenzyl)-3-[(4R)-6-ethyl-2,2-dioxido-3,4-dihydro-1H-isothiochromen-4-yl)amino]-2-hydroxypropyl]-4-(2-methoxyethyl)benzamide 789490-83-1P, N-[(1S,2R)-1-(3,5-Difluorobenzyl)-2-hydroxy-3-[(4R)-6-neopentyl-2,2-dioxido-3,4-dihydro-1H-isothiochromen-4-yl)amino]propyl]benzamide 789490-84-2P, N-[(1S,2R)-3-[(4R)-6-tert-Butoxy-2,2-dioxido-3,4-dihydro-1H-isothiochromen-4-yl)amino]-1-(3,5-difluorobenzyl)-2-hydroxypropyl]benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of 2-hydroxy-3-aminoalkylbenzamides as β-secretase inhibitors for treatment of Alzheimer's disease)

RN 527731-85-7 CAPLUS

CN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

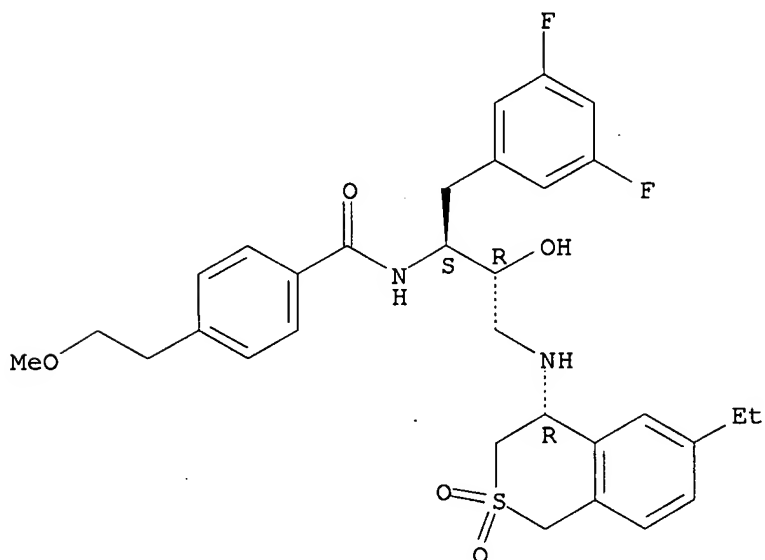
Absolute stereochemistry.



RN 527733-19-3 CAPLUS

CN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-4-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

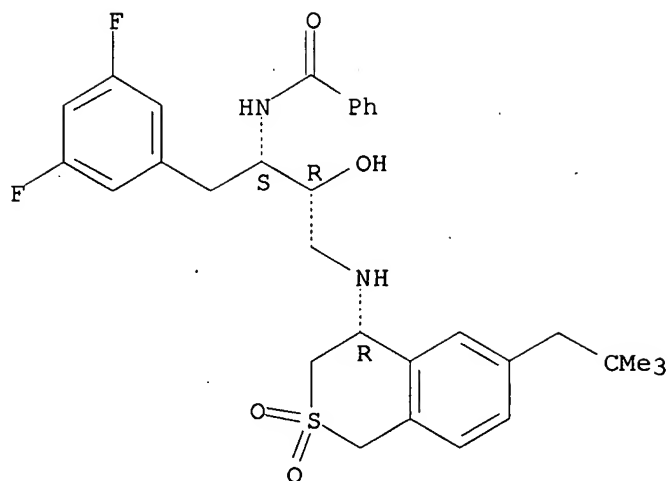
Absolute stereochemistry.



RN 789490-83-1 CAPLUS

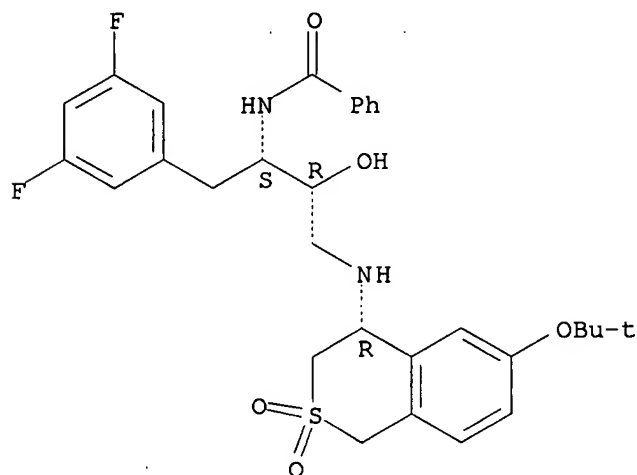
CN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-(2,2-dimethylpropyl)-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 789490-84-2 CAPLUS
 CN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-(1,1-dimethylethoxy)-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:493666 CAPLUS
 DN 141:23911
 TI Preparation of peptide-related substituted ureas and carbamates for the treatment of Alzheimer's disease
 PA Elan Pharmaceutical, Inc., USA; Pharmacia & Upjohn Company, LLC; Pulley, Shon R.; Tucker, John A.
 SO PCT Int. Appl., 213 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004050609	A1	20040617	WO 2003-US37998	20031126
	WO 2004050609	A8	20050721		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2507484	A1	20040617	CA 2003-2507484	20031126
AU 2003293155	A1	20040623	AU 2003-293155	20031126
US 2004209925	A1	20041021	US 2003-723220	20031126
EP 1565428	A1	20050824	EP 2003-790144	20031126

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

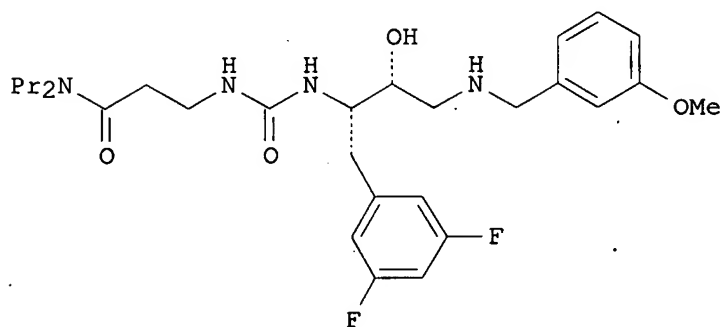
BR 2003016629	A	20051011	BR 2003-16629	20031126
JP 2006508166	T	20060309	JP 2004-557383	20031126

PRAI US 2002-429769P P 20021127

WO 2003-US37998 W 20031126

OS MARPAT 141:23911

GI



AB The invention provides compds. RN-T-X-NR20CHR1CH(OH)CR2R3NR20RC [X is CO, CS, S, SO, SO2 or C:N-Z, where Z is R20 or OR20; T is absent, NR20 or O; R20 is H, CN, alk(en)yl, haloalkyl or cycloalkyl; R1 is (CH2)1-2S(O)0-2-alkyl, (un)substituted alk(en)(yn)yl, (hetero)aryl, heterocyclyl, , etc.; RC, RN are (un)substituted alkyl, (hetero)aryl, heterocyclyl, etc.; R2, R3 are H or (un)substituted alkyl (with provisos)] which are inhibitors of the β -secretase enzyme and are useful in the treatment of Alzheimer's disease and related diseases. Thus, compound I was prepared by ring opening of tert-Bu (1S)-2-(3,5-difluorophenyl)-1-[(2S)-oxiran-2-yl]ethylcarbamate with 3-methoxybenzylamine, deprotection with TFA, reaction with the product generated from Pr2NCOCH2CH2CO2H, Et3N and (PhO)2P(O)N3, and deprotection.

IT 700866-46-2P 700866-47-3P 700866-48-4P
700866-49-5P 700866-50-8P 700866-51-9P
700866-52-0P

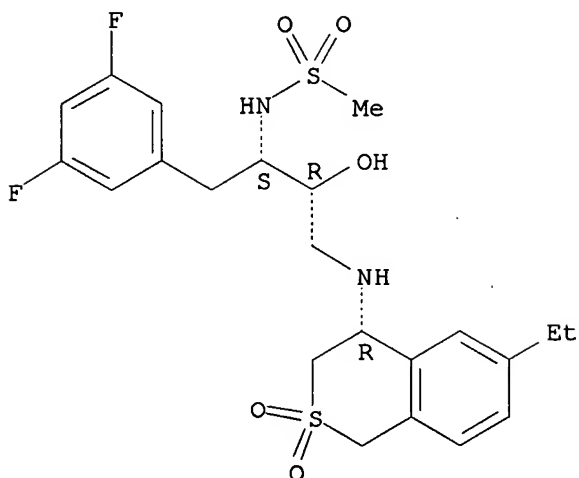
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of peptide-related substituted ureas and carbamates for treatment of Alzheimer's disease)

RN 700866-46-2 CAPLUS

CN Methanesulfonamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

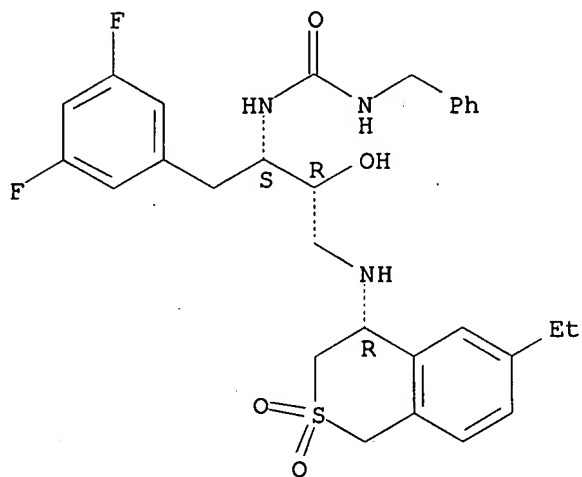
Absolute stereochemistry.



RN 700866-47-3 CAPLUS

CN Urea, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)

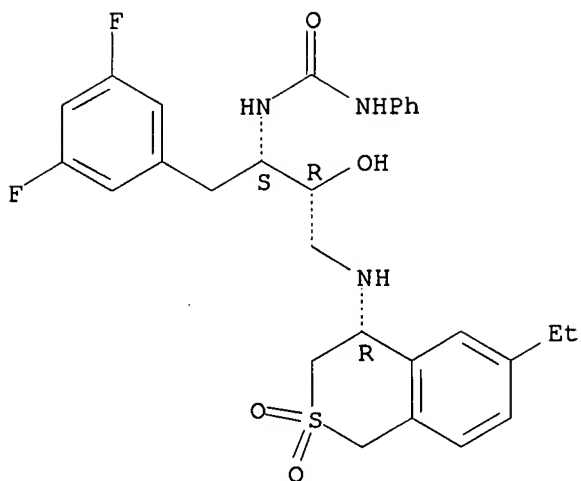
Absolute stereochemistry.



RN 700866-48-4 CAPLUS

CN Urea, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-N'-phenyl- (9CI) (CA INDEX NAME)

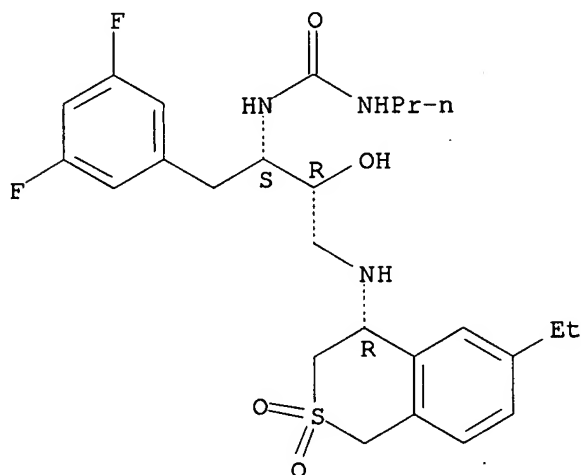
Absolute stereochemistry.



RN 700866-49-5 CAPLUS

CN Urea, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-N'-propyl- (9CI) (CA INDEX NAME)

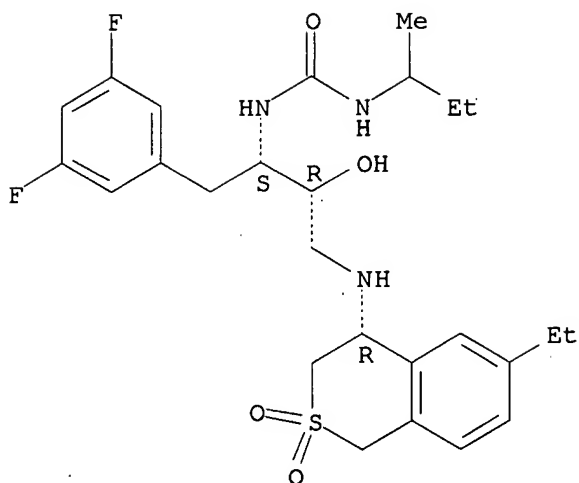
Absolute stereochemistry.



RN 700866-50-8 CAPLUS

CN Urea, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-N'-(1-methylpropyl)- (9CI) (CA INDEX NAME)

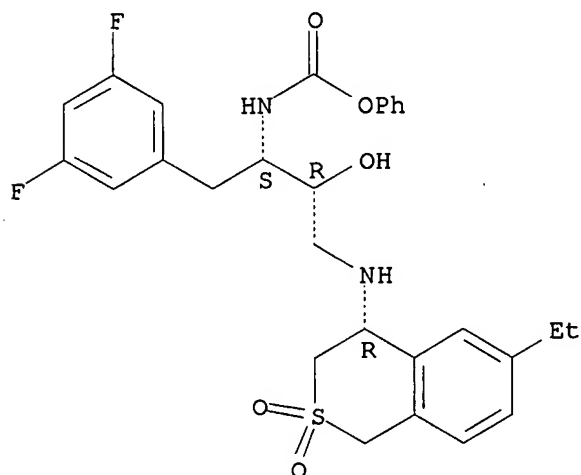
Absolute stereochemistry.



RN 700866-51-9 CAPLUS

CN Carbamic acid, [(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-, phenyl ester (9CI) (CA INDEX NAME)

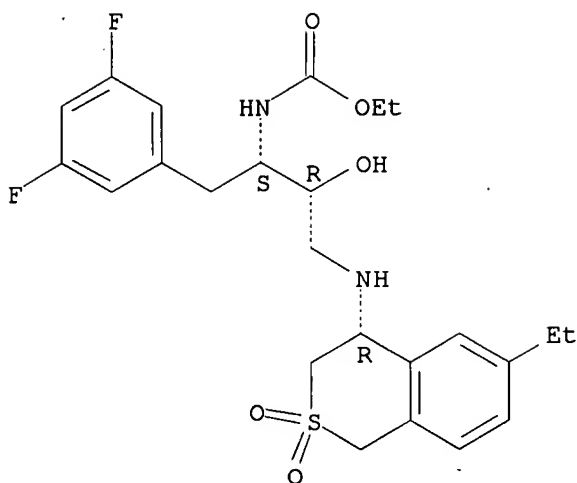
Absolute stereochemistry.



RN 700866-52-0 CAPLUS

CN Carbamic acid, [(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



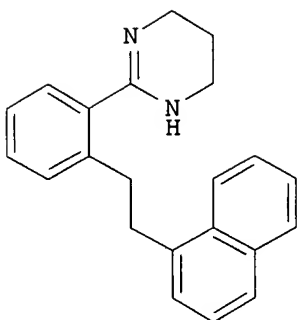
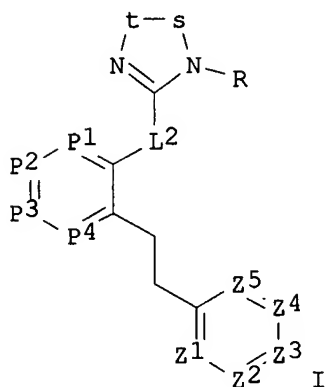
RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:353186 CAPLUS
DN 140:375177
TI Preparation of melanocortin-4 receptor binding compounds
IN Vos, Tricia J.; Solomon, Michael E.; Claiborne, Christopher F.; Maguire, Martin P.; Dai, Mingshi; Patane, Michael; Marsilje, Thomas H.
PA Millennium Pharmaceuticals, Inc., USA
SO U.S. Pat. Appl. Publ., 299 pp., Cont.-in-part of U.S. 6,699,873.
CODEN: USXXCO

DT Patent
LA English

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004082779	A1	20040429	US 2003-462436	20030616
	US 6699873	B1	20040302	US 2001-778468	20010207
	CA 2529445	A1	20051222	CA 2004-2529445	20040615
	WO 2005121100	A1	20051222	WO 2004-US19124	20040615
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	US 2000-223277P	P	20000803		
	US 2000-632309	B2	20000804		
	US 2001-778468	A2	20010207		
	US 2003-462436	A	20030616		
	WO 2004-US19124	W	20040615		



II

AB The title compds. of formula B-Z-E [wherein B = an anchor moiety; Z = a central moiety; E = an MC4-R interacting moiety], e.g. I [wherein P1-P4 = (un)substituted C, wherein one of P1-R4 is optionally replaced by N atom, or the ring bearing P1-P4 is thiophene ring wherein P3R4 together are replaced by a S atom; Z1-Z5 = (un)substituted CH; L2 = a bond, (un)substituted C1-2 alkylene, 2 carbon carbonyl chain, wherein one of the carbons is optionally replaced by O, NH, S; t = CH2, CHR3, CR3R4; s = CH2, CHR5, CR5R6, or t-s taken together = CH:CH, CR3:CH, CH:CR5, CR3:CR5; R3-R6 = alkyl, alkylcarbonyl, alkoxyacrbonyl, etc.; R = H, alkyl, alkylcarbonyl], were prepared and tested as melanocortin-4 receptor (MC4-R) binding agonists and antagonists. For example, α -tolunitrile in THF was added to a solution of diisopropylamine in THF, which had been cooled to -78°C and treated with BuLi. HMPA and 1-chloromethylnaphthalene in THF were added, the reaction cooled and stirred for 1 h, and the reaction quenched with H2O to give 2-(2-naphthalen-1-ylethyl)benzonitrile. Treatment with H2S and 1,3-diaminopropane, followed by heating to 80°C for 72 h and work up, gave II. In a scintillation proximity assay (SPA) using high-throughput receptor binding screening, II showed exemplary inhibition of MC4-R. The invention compds., primarily 2-(2-arylalkylsulfanylphenyl)-4,5-dihydro-1H-imidazole and 1,4,5,6-tetrahydropyrimidine derivs., are useful in the treatment of disorders associated with weight loss (no data). The pharmaceutical composition

comprising the title compds. is claimed.

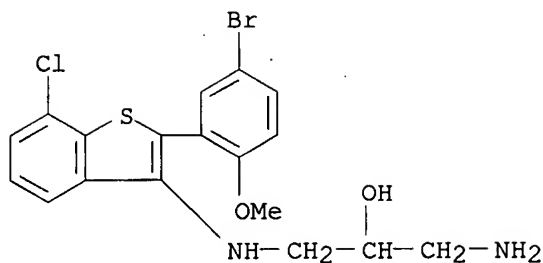
IT 447462-54-6P 447462-69-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

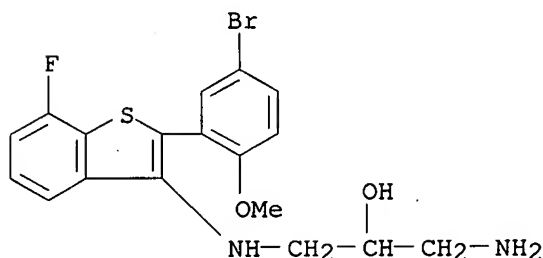
(preparation and high throughput MC4-R receptor binding screening of arylalkylsulfanylphenyl-substituted imidazoles and pyrimidines and analogs)

RN 447462-54-6 CAPLUS

CN 2-Propanol, 1-amino-3-[[2-(5-bromo-2-methoxyphenyl)-7-chlorobenzo[b]thien-3-yl]amino]- (9CI) (CA INDEX NAME)



RN 447462-69-3 CAPLUS
 CN 2-Propanol, 1-amino-3-[[2-(5-bromo-2-methoxyphenyl)-7-fluorobenzo[b]thien-3-yl]amino]- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:292015 CAPLUS
 DN 140:303413
 TI Preparation of hydroxyaminopropylbenzamides for the treatment of Alzheimer's disease
 IN Hom, Roy; Varghese, John
 PA Elan Pharmaceuticals, Inc., USA
 SO PCT Int. Appl., 117 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004029019	A2	20040408	WO 2003-US30388	20030926
	WO 2004029019	A3	20040527		
	WO 2004029019	A8	20050915		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	CA 2500109	A1	20040408	CA 2003-2500109	20030926
	AU 2003299101	A1	20040419	AU 2003-299101	20030926
	EP 1542964	A2	20050622	EP 2003-756871	20030926
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	BR 2003014714	A	20050802	BR 2003-14714	20030926
	JP 2006501282	T	20060112	JP 2004-539965	20030926

US 2006128786 A1 20060615 US 2005-529504 20051005
 PRAI US 2002-414287P P 20020927
 WO 2003-US30388 W 20030926

OS MARPAT 140:303413

AB RnR1NCH2CH(OH)CR2R3NRcR20 [R20 = H, alkyl, alkenyl, haloalkyl, cycloalkyl; R1 = (CH2)1-2SO0-2alkyl, (substituted) alkyl, alkenyl, alkynyl, aryl, cycloalkyl; Rc = H, (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, alkylaryl, alkylheteroaryl, etc.; R2, R3 = H, (substituted) alkyl; R2R3C = atoms to form a 3-7 membered (heterocyclyl) ring; Rn = ((substituted)) aryl, heteroaryl, aminocarbonyl, aryloxy carbonyl, arylsulfonyl, etc.], were prepared as β -secretase inhibitors (no data). Thus, N-(3,5-difluorobenzyl)-5-methyl-N-(R)-oxiranylmethyl-N',N'-dipropylisophthalamide (preparation given) was refluxed with 3-iodobenzylamine in Me2CHOH to give N-(3,5-difluorobenzyl)-N-[(2R)-2-hydroxy-3-[(3-iodobenzyl)amino]propyl]-5-methyl-N',N'-dipropylisophthalamide. The compds. of the invention are useful in pharmaceutical compns. and methods of treatment to reduce A beta peptide formation.

IT 676597-27-6P 676597-28-7P 676597-29-8P

676597-33-4P 676597-34-5P 676597-35-6P

676597-39-0P 676597-40-3P 676597-41-4P

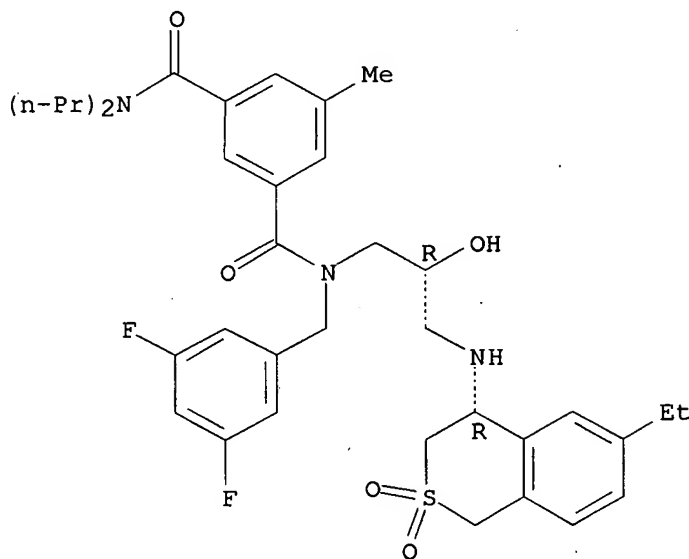
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of hydroxyaminopropylbenzamides for the treatment of Alzheimer's disease)

RN 676597-27-6 CAPLUS

CN 1,3-Benzenedicarboxamide, N-[(3,5-difluorophenyl)methyl]-N-[(2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N',N'-dipropyl- (9CI) (CA INDEX NAME)

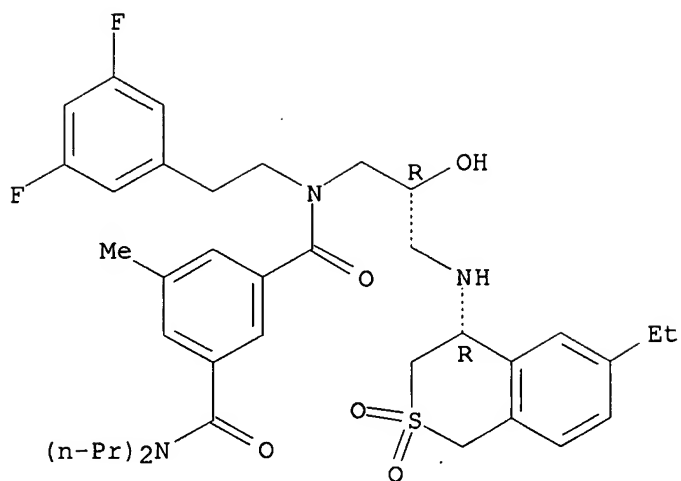
Absolute stereochemistry.



RN 676597-28-7 CAPLUS

CN 1,3-Benzenedicarboxamide, N-[2-(3,5-difluorophenyl)ethyl]-N-[(2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N',N'-dipropyl- (9CI) (CA INDEX NAME)

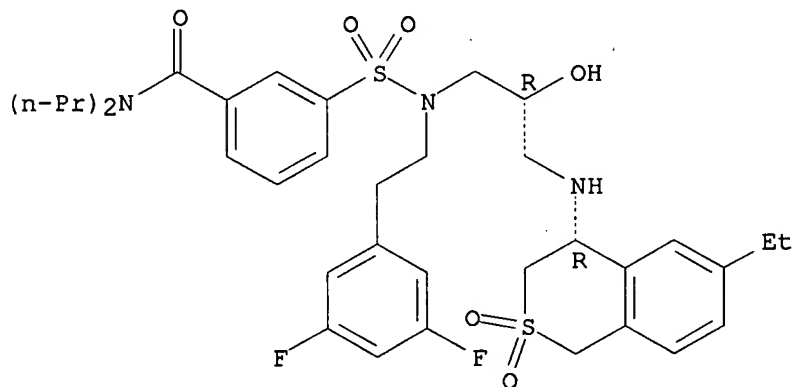
Absolute stereochemistry.



RN 676597-29-8 CAPLUS

CN Benzamide, 3-[[[2-(3,5-difluorophenyl)ethyl][(2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]amino]sulfonyl]-N,N-dipropyl- (9CI) (CA INDEX NAME)

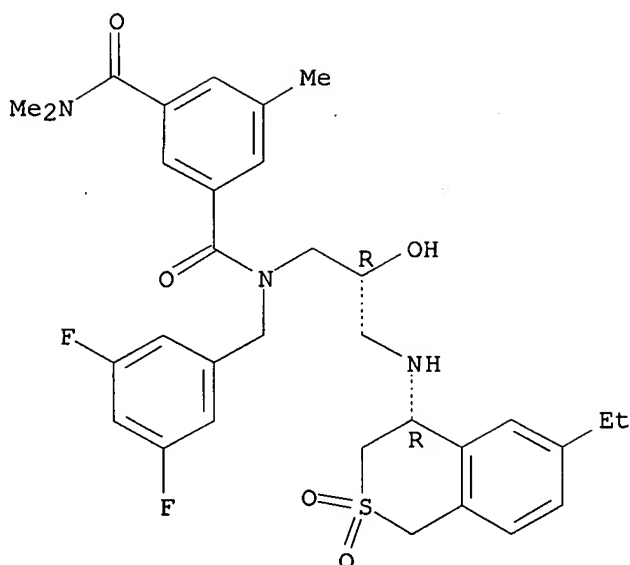
Absolute stereochemistry.



RN 676597-33-4 CAPLUS

CN 1,3-Benzenedicarboxamide, N-[(3,5-difluorophenyl)methyl]-N-[(2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-N',N',5-trimethyl- (9CI) (CA INDEX NAME)

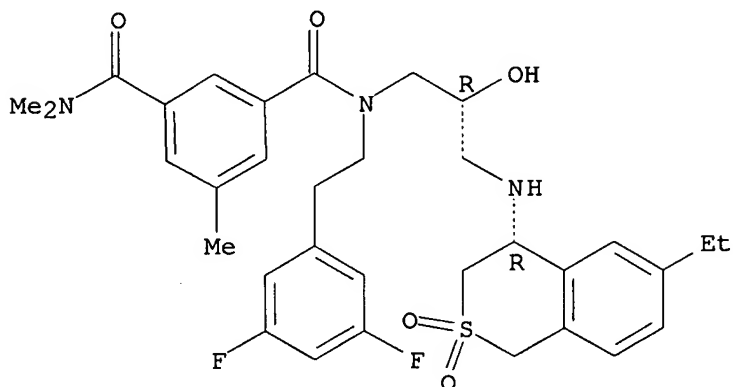
Absolute stereochemistry.



RN 676597-34-5 CAPLUS

CN 1,3-Benzenedicarboxamide, N-[2-(3,5-difluorophenyl)ethyl]-N-[(2R)-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-N',N',5-trimethyl- (9CI) (CA INDEX NAME)

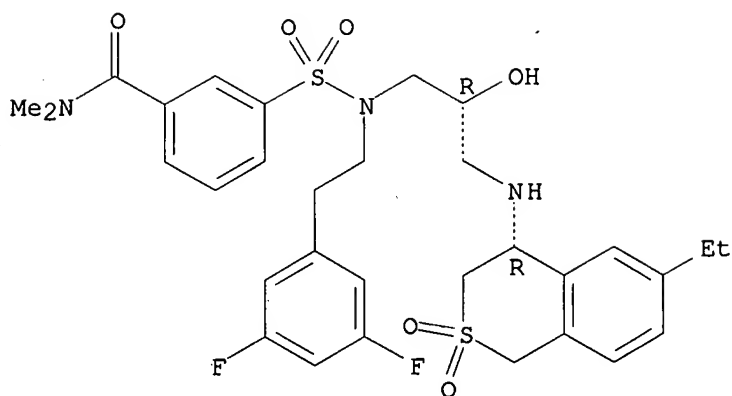
Absolute stereochemistry.



RN 676597-35-6 CAPLUS

CN Benzamide, 3-[[[2-(3,5-difluorophenyl)ethyl][(2R)-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]amino]sulfonyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

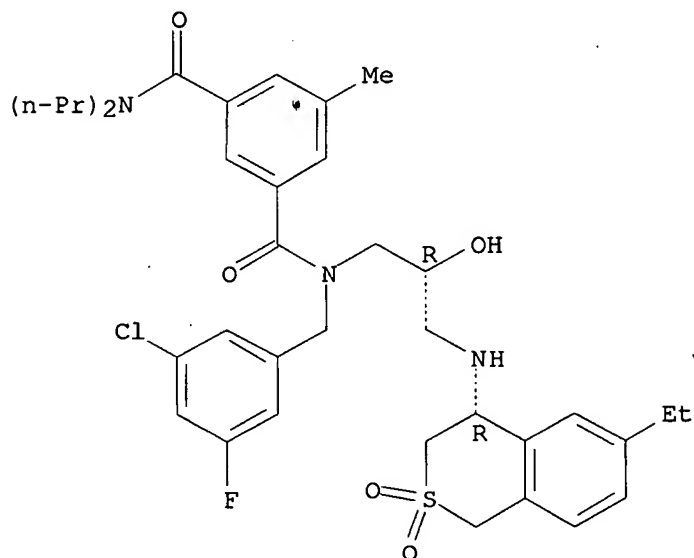
Absolute stereochemistry.



RN 676597-39-0 CAPLUS

CN 1,3-Benzenedicarboxamide, N-[(3-chloro-5-fluorophenyl)methyl]-N-[(2R)-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N',N'-dipropyl- (9CI) (CA INDEX NAME)

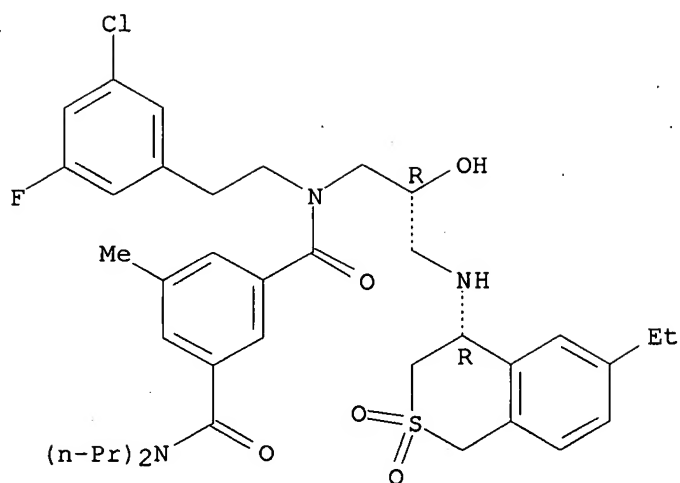
Absolute stereochemistry.



RN 676597-40-3 CAPLUS

CN 1,3-Benzenedicarboxamide, N-[2-(3-chloro-5-fluorophenyl)ethyl]-N-[(2R)-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N',N'-dipropyl- (9CI) (CA INDEX NAME)

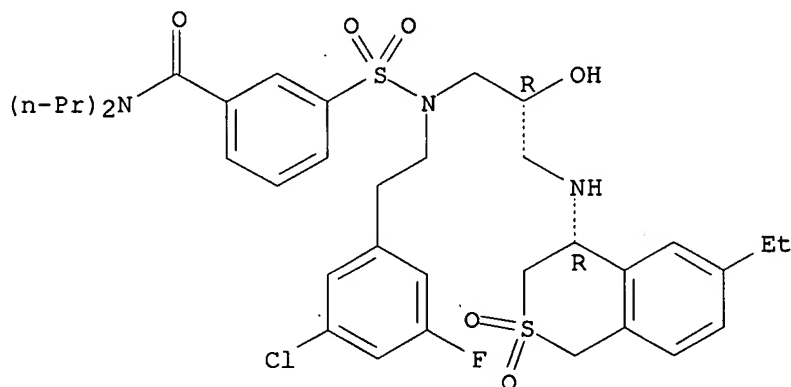
Absolute stereochemistry.



RN 676597-41-4 CAPLUS

CN Benzamide, 3-[[[2-(3-chloro-5-fluorophenyl)ethyl][(2R)-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]amino]sulfonyl]-N,N-dipropyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:252298 CAPLUS

DN 140:287268

TI Preparation of ring-containing N-acetyl 2-hydroxy-1,3-diaminoalkanes as β -secretase inhibitors for treating Alzheimer's disease and other diseases characterized by deposition of A β -peptide

IN Maillard, Michel; Baldwin, Eric T.; Beck, James T.; Hughes, Robert; John, Varghese; Pulley, Shon R.; Tenbrink, Ruth

PA Elan Pharmaceuticals, Inc., USA; Pfizer, Inc.; Pharmacia & Upjohn Company, LLC

SO PCT Int. Appl., 459 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004024081	A2	20040325	WO 2003-US28503	20030910
	WO 2004024081	A3	20050623		

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2498248	A1	20040325	CA 2003-2498248	20030910
AU 2003267132	A1	20040430	AU 2003-267132	20030910
US 2004180939	A1	20040916	US 2003-658959	20030910
BR 2003014188	A	20050809	BR 2003-14188	20030910
EP 1565443	A2	20050824	EP 2003-749607	20030910

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

CN 1694870	A	20051109	CN 2003-824988	20030910
JP 2006504793	T	20060209	JP 2004-571986	20030910
NZ 539095	A	20070427	NZ 2003-539095	20030910
NO 2005001239	A	20050606	NO 2005-1239	20050310
IN 2005KN00409	A	20060421	IN 2005-KN409	20050314
ZA 2005001991	A	20050309	ZA 2005-1991	20051020

PRAI US 2002-409453P P 20020910

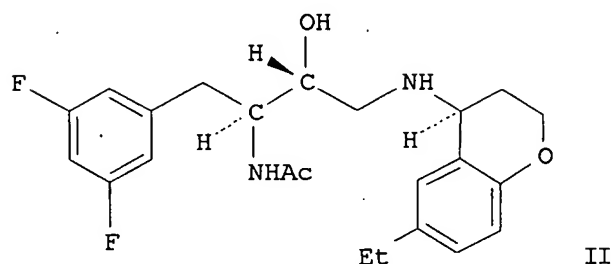
US 2003-452231P P 20030305

US 2003-491757P P 20030801

WO 2003-US28503 W 20030910

OS MARPAT 140:287268

GI



AB Disclosed are Z-X-NHCH(R1)CH(OH)C(R2)(R3)N(R15)(Rc) (I; variables defined below; e.g. II). Compds. disclosed herein are inhibitors of the beta-secretase enzyme (no data) and are therefore useful in the treatment of Alzheimer's disease and other diseases characterized by deposition of A beta peptide in a mammal (no data). An unspecified method of preparation is claimed and >100 example preps. of intermediates and I are included. For example, II was prepared in 4 steps starting with preparation of (6-iodochroman-4-yl)amine from 6-iodo-4-chroman-4-ol followed by reaction with tert-Bu [(1S)-2-(3,5-difluorophenyl)-1-((2S)-oxiran-2-yl)ethyl]carbamate to give tert-Bu [(1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-3-[(6-iodo-3,4-dihydro-2H-chromen-4-yl)aminopropyl]carbamate, followed by ethylation. For I: Z is H, (C3-C7 cycloalkyl)O-1(C1-C6 alkyl)-, (C3-C7 cycloalkyl)O-1(C2-C6 alkenyl)-, (C3-C7 cycloalkyl)O-1(C2-C6 alkynyl)- or (C3-C7 cycloalkyl)-; X = C(O), SO₂; R1 is C1-C10 alkyl (un)substituted with 1, 2, or 3 halogen, -OH, -O-, -SH, -CN, -CF₃, -OCF₃, -C3-7 cycloalkyl, -C1-C4 alkoxy, amino, mono- or dialkylamino, aryl, heteroaryl, and heterocycloalkyl; R2 and R3 = H; F; -C1-C6 alkyl (un)substituted with -F, -OH, -CN, -CF₃, C1-C3 alkoxy, or -NR₅R₆; -(CH₂)₀₋₂-R17; -(CH₂)₀₋₂-R18; -C2-C6 alkenyl or C2-C6 alkynyl;.

R15 = H, C1-C6 alkyl, C1-C6 alkoxy, C1-C6 alkoxy C1-C6 alkyl, hydroxy C1-C6 alkyl, halo C1-C6 alkyl; R2, R3 and the C to which they are attached can form a C3-C7 carbocycle, wherein 1-3 C atoms are optionally replaced by -O-, -S-, -SO2-, -C(O)-, or -NR7-; Rc = -(CH2)0-3-(C3-C8) cycloalkyl, etc.; addnl. details are given in the claims.

IT 527730-68-3P 527730-69-4P 527731-50-6P
 676133-51-0P 676133-52-1P 676133-53-2P
 676133-54-3P 676133-55-4P 676133-56-5P
 676133-57-6P 676133-58-7P 676133-59-8P
 676133-60-1P 676133-61-2P 676135-54-9P
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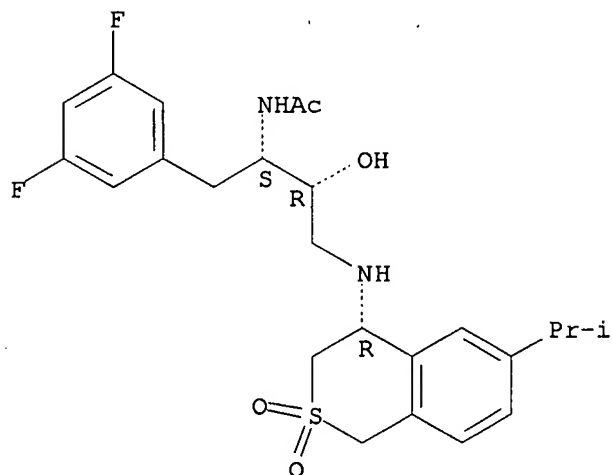
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of ring-containing N-acetyl 2-hydroxy-1,3-diaminoalkanes as β -secretase inhibitors for treating Alzheimer's disease and other diseases characterized by deposition of A β -peptide)

RN 527730-68-3 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

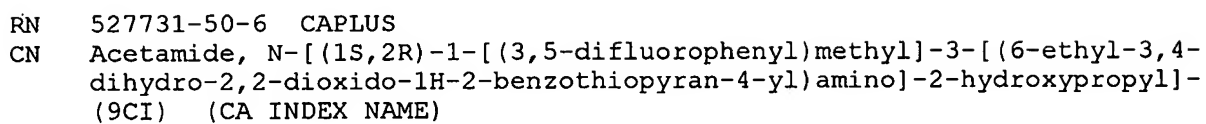
Absolute stereochemistry.



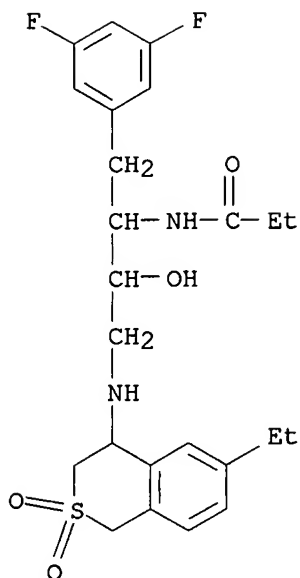
RN 527730-69-4 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

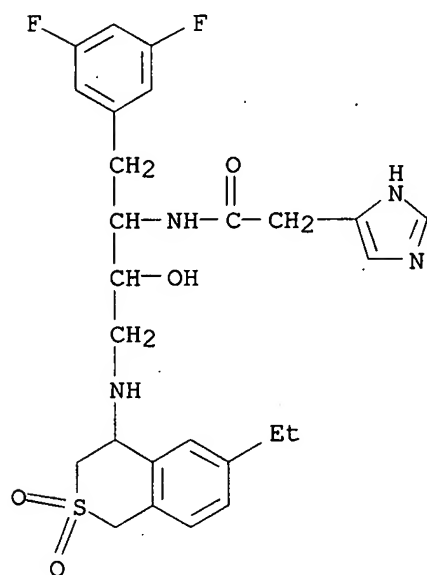
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RN 676133-51-0 CAPLUS
CN Propanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)



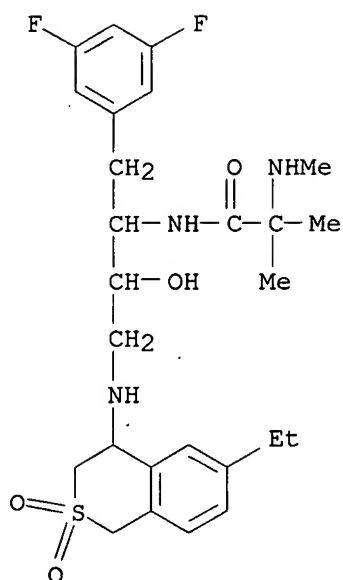
RN 676133-52-1 CAPLUS

CN 1H-Imidazole-4-acetamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)



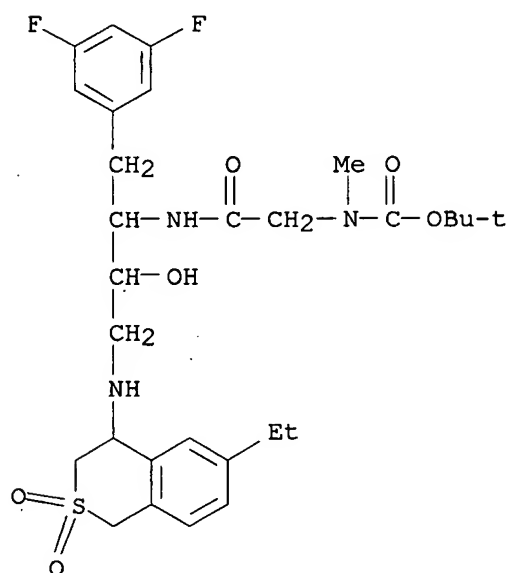
RN 676133-53-2 CAPLUS

CN Propanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-2-methyl-2-(methylamino)- (9CI) (CA INDEX NAME)



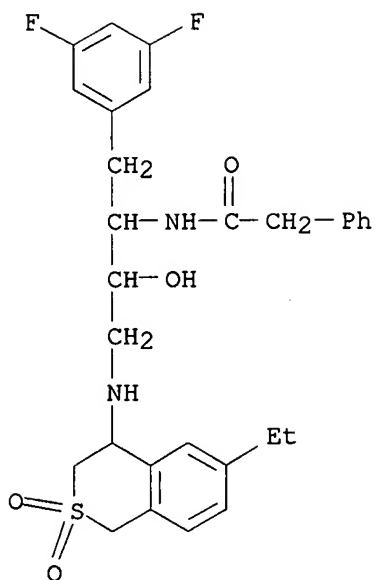
RN 676133-54-3 CAPLUS

CN Carbamic acid, [2-[[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]amino]-2-oxoethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



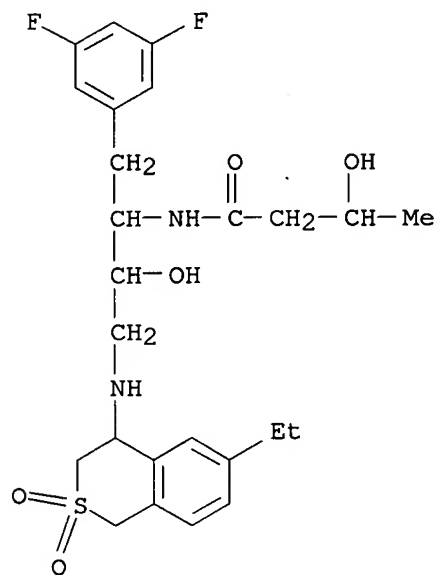
RN 676133-55-4 CAPLUS

CN Benzeneacetamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)



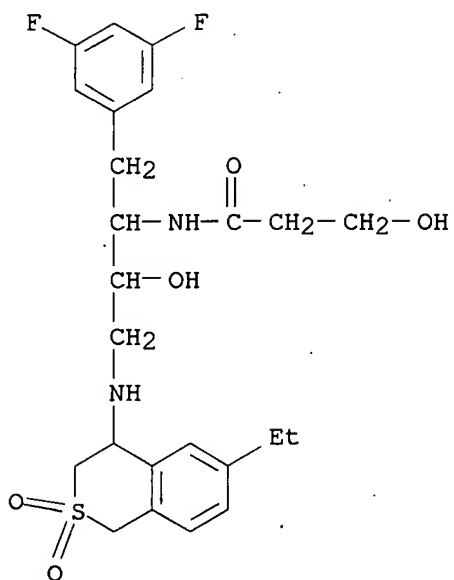
RN 676133-56-5 CAPLUS

CN Butanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3-hydroxy- (9CI)
(CA INDEX NAME)



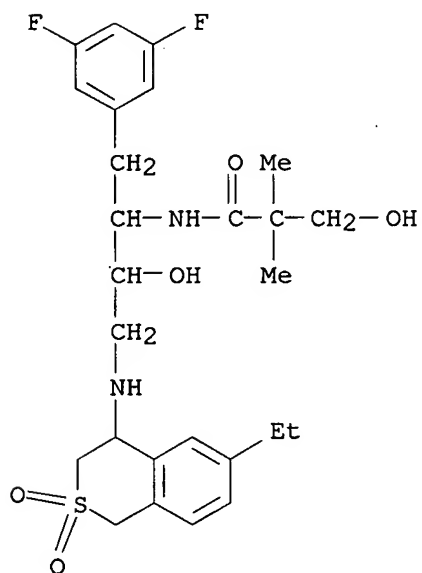
RN 676133-57-6 CAPLUS

CN Propanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3-hydroxy- (9CI)
(CA INDEX NAME)



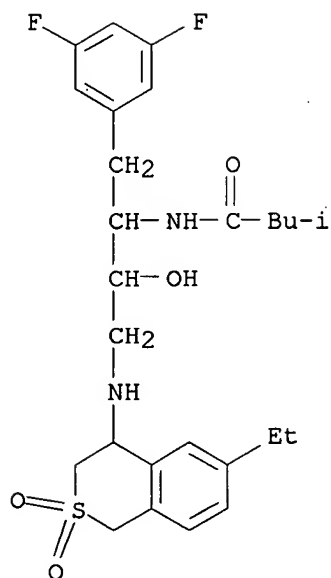
RN 676133-58-7 CAPLUS

CN Propanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3-hydroxy-2,2-dimethyl- (9CI) (CA INDEX NAME)



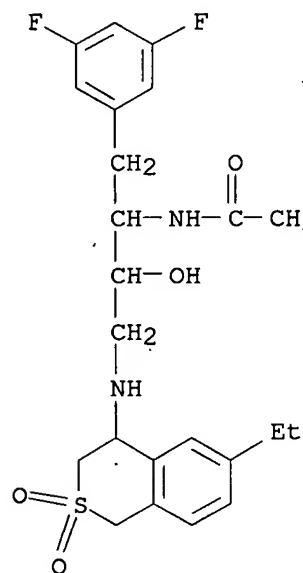
RN 676133-59-8 CAPLUS

CN Butanamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-3-methyl- (9CI) (CA INDEX NAME)



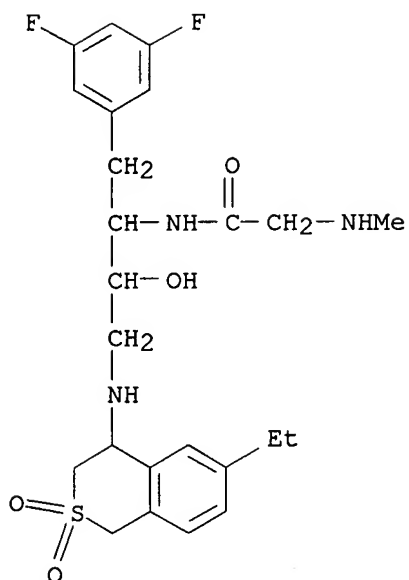
RN 676133-60-1 CAPLUS

CN Acetamide, 2-amino-N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-
(9CI) (CA INDEX NAME)



RN 676133-61-2 CAPLUS

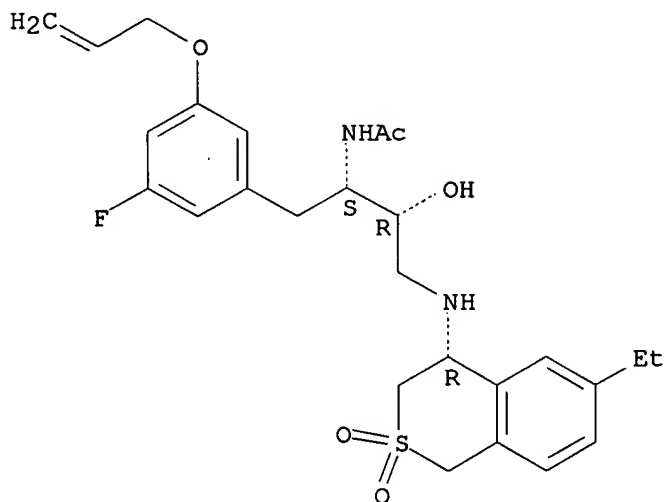
CN Acetamide, N-[1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-2-(methylamino)-
(9CI) (CA INDEX NAME)



RN 676135-54-9 CAPLUS

CN Acetamide, N-[(1S,2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-1-[[3-fluoro-5-(2-propenyloxy)phenyl]methyl]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

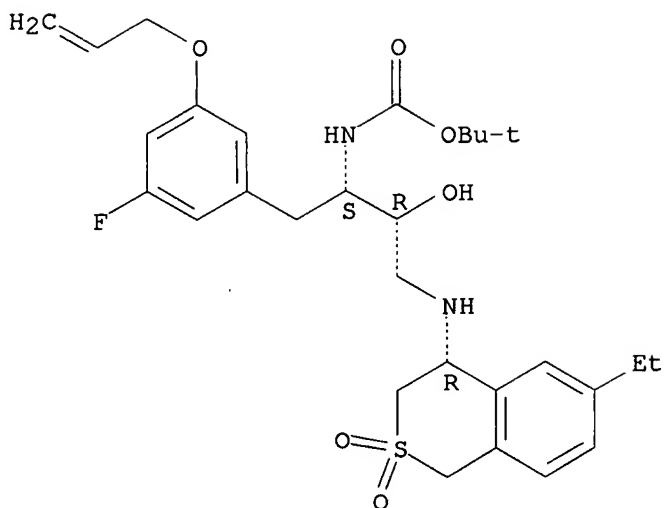
Absolute stereochemistry.



RN 676135-56-1 CAPLUS

CN Carbamic acid, [(1S,2R)-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-1-[[3-fluoro-5-(2-propenyloxy)phenyl]methyl]-2-hydroxypropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

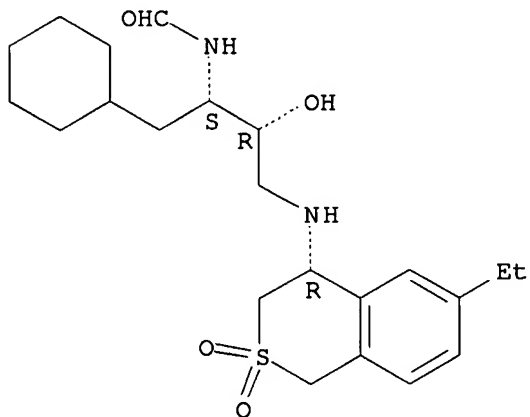
Absolute stereochemistry.



RN 676135-57-2 CAPLUS

CN Formamide, N-[(1S,2R)-1-(cyclohexylmethyl)-3-[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

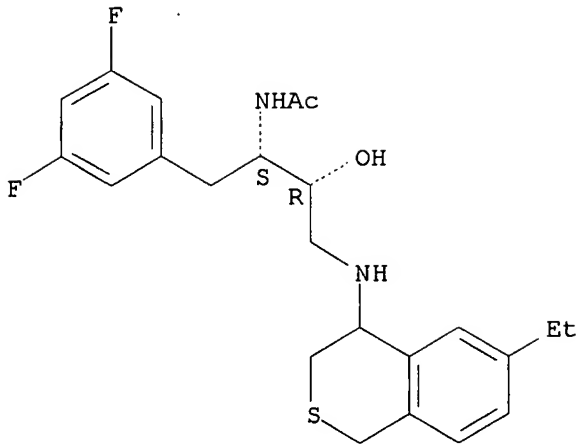
Absolute stereochemistry.



RN 676138-56-0 CAPLUS

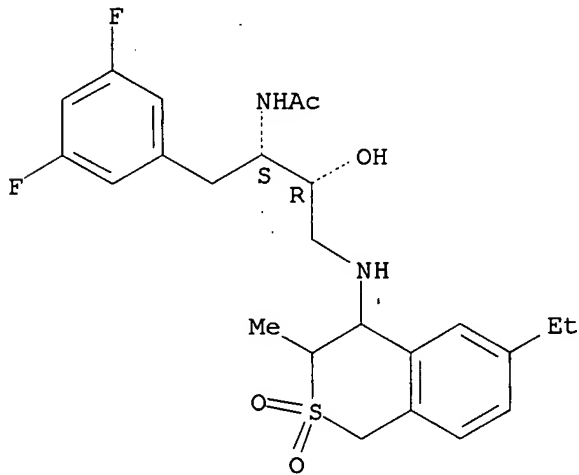
CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676138-65-1 CAPLUS
 CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-3-methyl-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

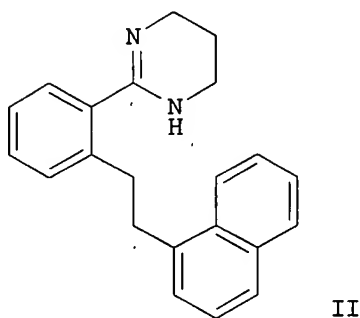
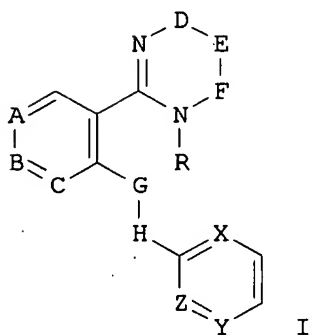


L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:176560 CAPLUS
 DN 140:217656
 TI Preparation of aryl-substituted tetrahydropyrimidines and related compounds as melanocortin-4 receptor binding compounds
 IN Maguire, Martin P.; Dai, Mingshi; Vos, Tricia J.
 PA Millennium Pharmaceuticals, Inc., USA
 SO U.S., 216 pp., Cont.-in-part of U.S. Ser. No. 632309.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6699873	B1	20040302	US 2001-778468	20010207
	WO 2002062766	A2	20020815	WO 2002-US3566	20020207
	WO 2002062766	A3	20021003		

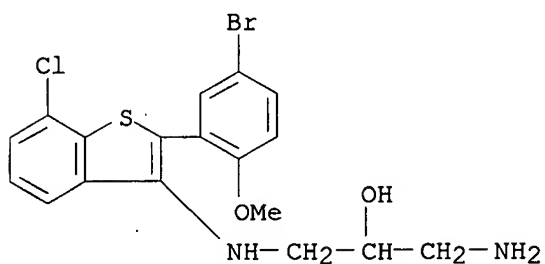
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 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 AU 2002250029 A1 20020819 AU 2002-250029 20020207
 EP 1363890 A2 20031126 EP 2002-718920 20020207
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 US 2004082779 A1 20040429 US 2003-462436 20030616
 PRAI US 1999-147288P P 19990804
 US 2000-223277P P 20000803
 US 2000-632309 A2 20000804
 US 2001-778468 A 20010207
 WO 2002-US3566 W 20020207
 OS MARPAT 140:217656
 GI

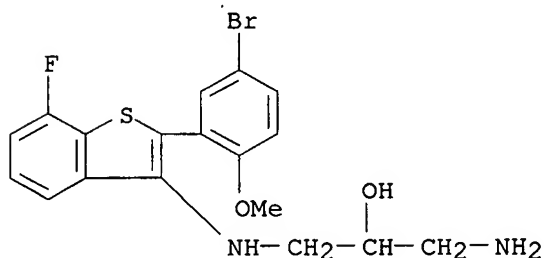


- AB The title compds. [I and related compds.; A = CH, CF, CCl, C(alkyl), etc.; B = CH, CF, CCl, C(alkyl), etc.; C = CH, CCl, S, etc.; G, H = CH₂, S; D = CH₂; E, F = (un)substituted CH₂; X = C(alkoxy); Y = CH, C(C.tplbond.CH), CCl, CBr, CCl, CF; Z = CH; or pharmaceutically acceptable salts thereof] were prepared for treating a melanocortin-4 receptor (MC4-R) associated state in a mammal. For example, stirring a solution of α -tolunitrile with diisopropylamine and BuLi in hexanes at -78° under nitrogen for 1 h, followed by addition of HMPA and 1-chloromethylnaphthalene in THF, afforded 2-(2-naphthalen-1-ylethyl)benzonitrile. Heating the benzonitrile with 1,3-diaminopropane in the presence of H₂S at 80° for 72 h gave the tetrahydropyrimidinyl cycloaddn. product II. The latter exhibited exemplary inhibition of MC4-R in a scintillation proximity assay. I are useful for the treatment of disorders associated with pigmentation, bones, or weight loss (no data).
- IT 447462-54-6P, 1-Amino-3-[2-(5-bromo-2-methoxyphenyl)-7-chlorobenzo[b]thiophen-3-ylamino]propan-2-ol 447462-69-3P, 1-Amino-3-[2-(5-bromo-2-methoxyphenyl)-7-fluorobenzo[b]thiophen-3-ylamino]propan-2-ol
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (MC4-R binding compound; preparation of aryl-substituted tetrahydropyrimidines and related compds. as melanocortin-4 receptor binding compds. for treatment of pigmentation, bone, and weight loss disorders)

RN 447462-54-6 CAPLUS
 CN 2-Propanol, 1-amino-3-[[2-(5-bromo-2-methoxyphenyl)-7-chlorobenzo[b]thien-3-yl]amino]- (9CI) (CA INDEX NAME)



RN 447462-69-3 CAPLUS
 CN 2-Propanol, 1-amino-3-[[2-(5-bromo-2-methoxyphenyl)-7-fluorobenzo[b]thien-3-yl]amino]- (9CI) (CA INDEX NAME)

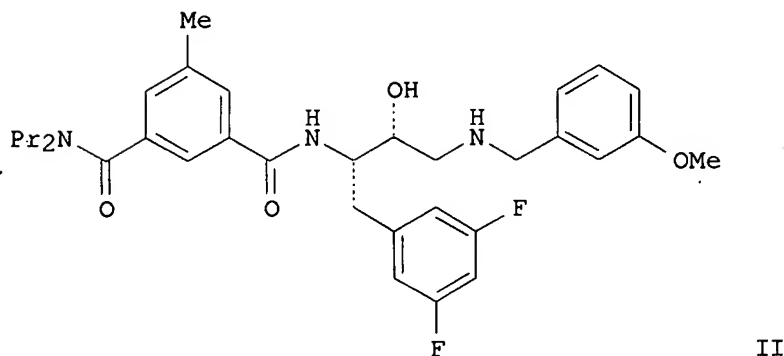
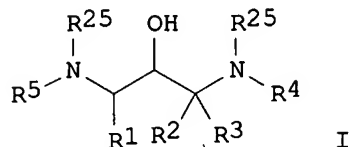


RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2003:412801 CAPLUS
 DN 139:245782
 TI Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease
 IN Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy
 PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
 SO PCT Int. Appl., 1243 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003040096	A2	20030515	WO 2002-XA36072	20021108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

WO 2003040096 A2 20030515 WO 2002-US36072 20021108
 WO 2003040096 A3 20040506
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 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
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 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
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 CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 ZA 2004003578 A 20051010 ZA 2004-3578 20040511
 PRAI US 2001-337122P P 20011108
 US 2001-344086P P 20011228
 US 2002-345635P P 20020103
 WO 2002-US36072 A 20021108
 OS MARPAT 139:245782
 GI



AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.;
 R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl,
 alkenyl, etc.; or R2 and R3 are taken together with the carbon to which
 they are attached to form a carbocycle of 3-7 carbon atoms, optionally
 where one carbon atom is replaced by a heteroatom selected from the group
 consisting of O, S, SO₂, (un)substituted NH; R4 = alkyl, haloalkyl,
 hydroxyalkyl, etc.; R5 = R₆X (wherein X = CO, SO₂, (un)substituted CH₂; R₆
 = (un)substituted Ph, naphthyl, indanyl, etc.); R₂₅ = H, alkyl, alkoxy,
 etc.] which have activity as inhibitors of β -secretase and are
 therefore useful in treating a variety of disorders such as Alzheimer's
 disease, were prepared E.g., a multi-step synthesis of (1S,2R)-II, starting
 from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic
 acid, was given. The compds. I showed IC₅₀ of < 20 μ M in cell free
 inhibition assay utilizing a synthetic APP substrate. This is a Part 2 of
 1-2 series.

IT 527731-85-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

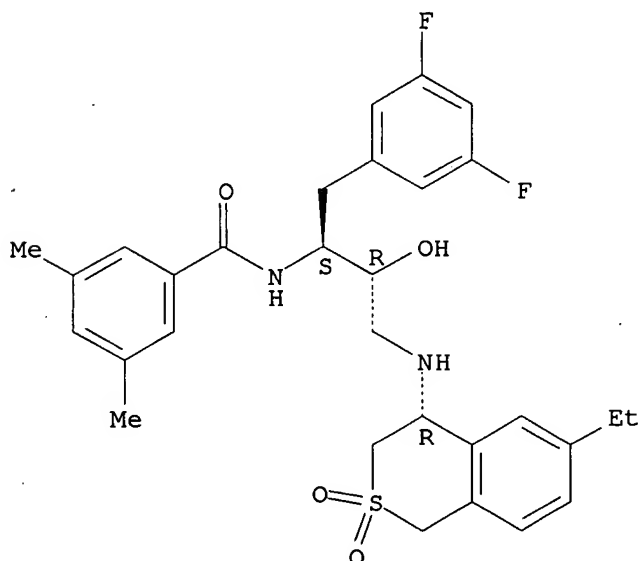
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease)

RN 527731-85-7 CAPLUS

CN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:376819 CAPLUS

DN 138:385173

TI Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease

IN Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy

PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company

SO PCT Int. Appl., 1243 pp.

CODEN: PIXXD2

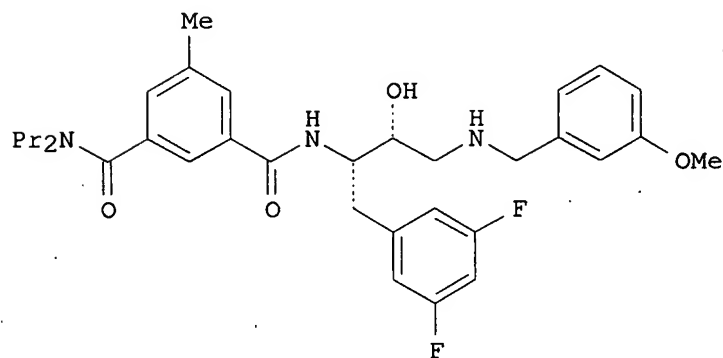
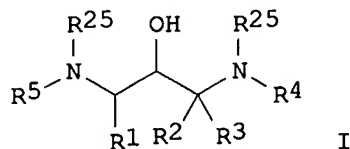
DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	WO 2003040096	A3	20040506		
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CA 2466284	A1	20030515	CA 2002-2466284	20021108
WO 2003040096	A2	20030515	WO 2002-XA36072	20021108
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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US 2004171881	A1	20040902	US 2002-291318	20021108
US 7176242	B2	20070213		
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NZ 533107	A	20070427	NZ 2002-533107	20021108
ZA 2004003578	A	20051010	ZA 2004-3578	20040511
IN 2004KN00627	A	20060224	IN 2004-KN627	20040514
NO 2004002359	A	20040806	NO 2004-2359	20040607
PRAI US 2001-337122P	P	20011108		
US 2001-344086P	P	20011228		
US 2002-345635P	P	20020103		
WO 2002-US36072	W	20021108		
OS MARPAT 138:385173				
GI				



AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, etc.; or R2 and R3 are taken together with the carbon to which

they are attached to form a carbocycle of 3-7 carbon atoms, optionally where one carbon atom is replaced by a heteroatom selected from the group consisting of O, S, SO₂, (un)substituted NH; R₄ = alkyl, haloalkyl, hydroxyalkyl, etc.; R₅ = R₆X (wherein X = CO, SO₂, (un)substituted CH₂; R₆ = (un)substituted Ph, naphthyl, indanyl, etc.); R₂₅ = H, alkyl, alkoxy, etc.] which have activity as inhibitors of β -secretase and are therefore useful in treating a variety of disorders such as Alzheimer's disease, were prepared. E.g., a multi-step synthesis of (1S,2R)-II, starting from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic acid, was given. The compds. I showed IC₅₀ of < 20 μ M in cell free inhibition assay utilizing a synthetic APP substrate. This is a Part 1 of 1-2 series.

IT 527712-34-1P 527712-36-3P 527712-38-5P
 527712-39-6P 527712-41-0P 527712-43-2P
 527712-45-4P 527712-47-6P 527712-49-8P
 527712-51-2P 527728-78-5P 527730-04-7P
 527730-68-3P 527730-69-4P 527731-50-6P
 527731-85-7P 527732-28-1P 527732-54-3P
 527732-55-4P 527732-56-5P 527732-57-6P
 527732-58-7P 527732-59-8P 527732-60-1P
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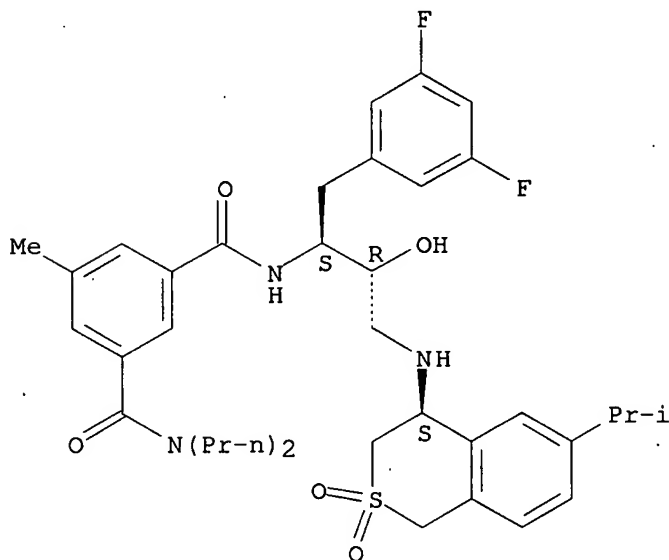
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease)

RN 527712-34-1 CAPLUS

CN 1,3-Benzenedicarboxamide, N'--[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

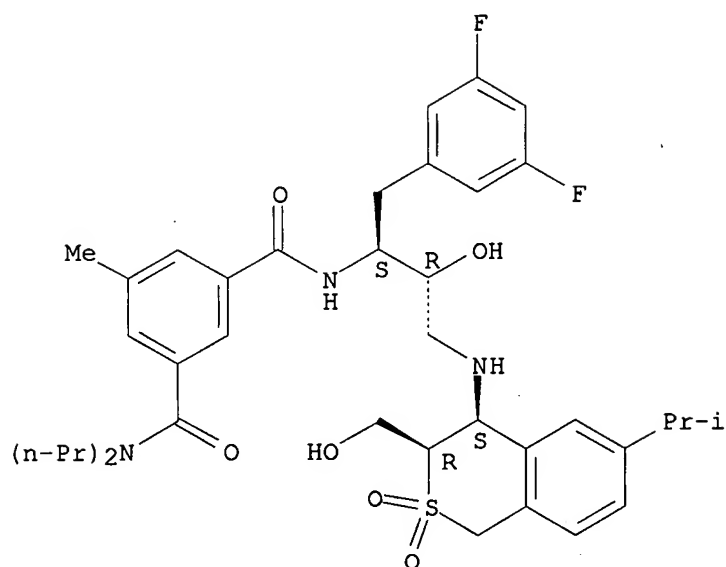


RN 527712-36-3 CAPLUS

CN 1,3-Benzenedicarboxamide, N'--[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3R,4S)-3,4-dihydro-3-(hydroxymethyl)-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)

(CA INDEX NAME)

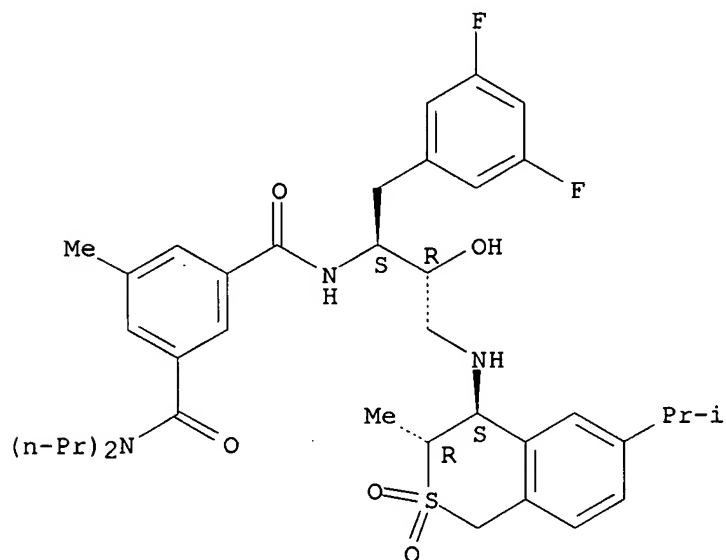
Absolute stereochemistry.



RN 527712-38-5 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3R,4S)-3,4-dihydro-3-methyl-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
(CA INDEX NAME)

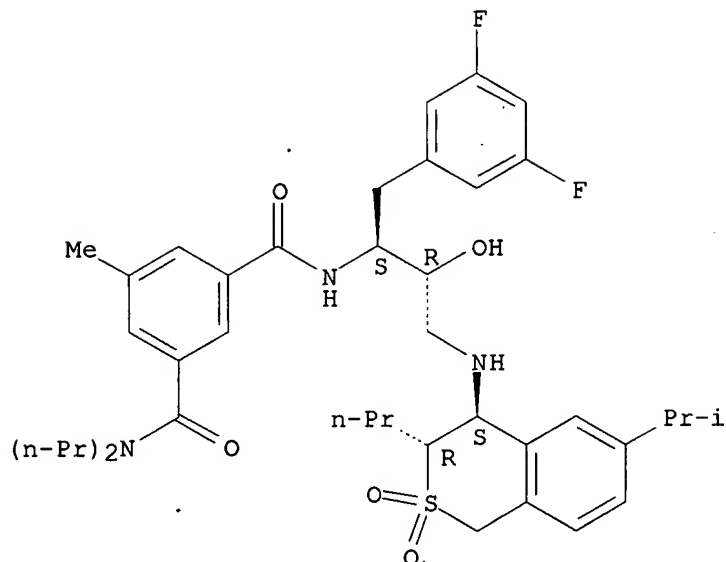
Absolute stereochemistry.



RN 527712-39-6 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3R,4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-3-propyl-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
(CA INDEX NAME)

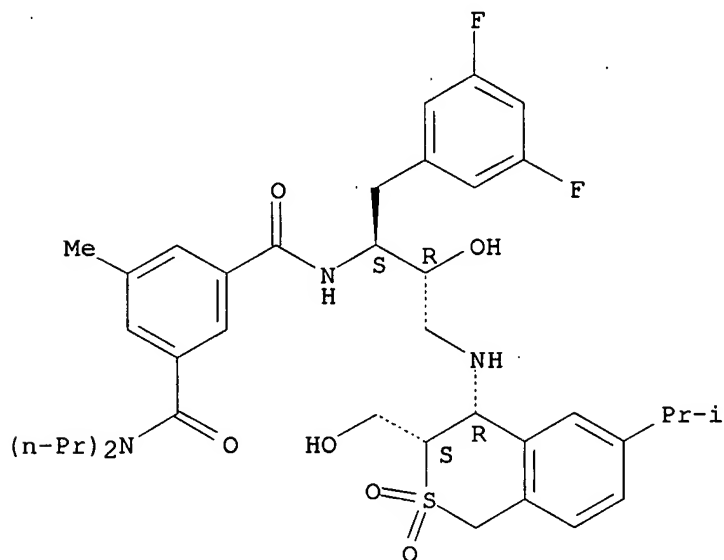
Absolute stereochemistry.



RN 527712-41-0 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3S,4R)-3,4-dihydro-3-(hydroxymethyl)-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
(CA INDEX NAME)

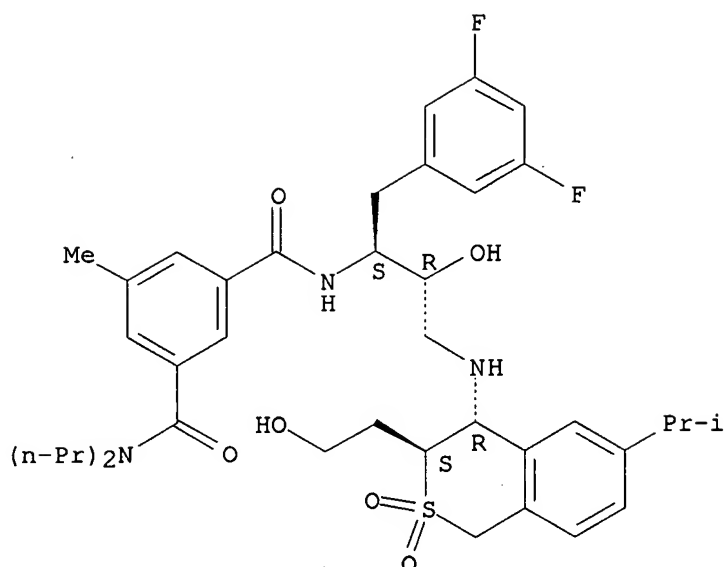
Absolute stereochemistry.



RN 527712-43-2 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3S,4R)-3,4-dihydro-3-(2-hydroxyethyl)-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
(CA INDEX NAME)

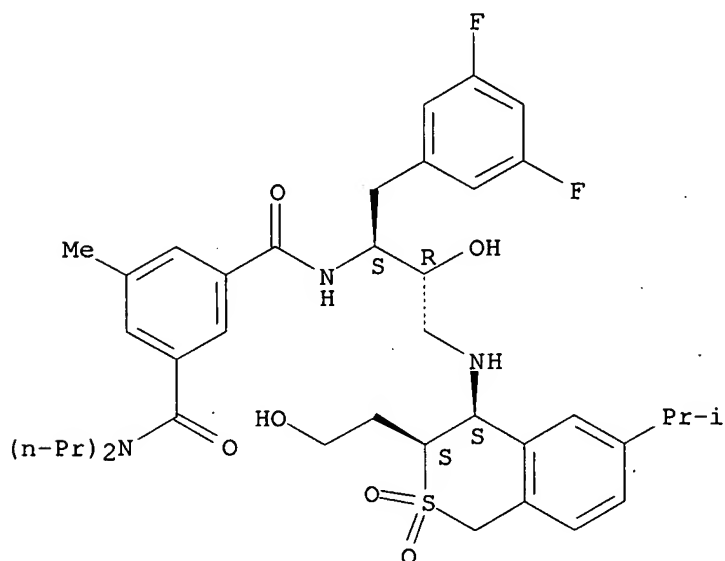
Absolute stereochemistry.



RN 527712-45-4 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3S,4S)-3,4-dihydro-3-(2-hydroxyethyl)-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
(CA INDEX NAME)

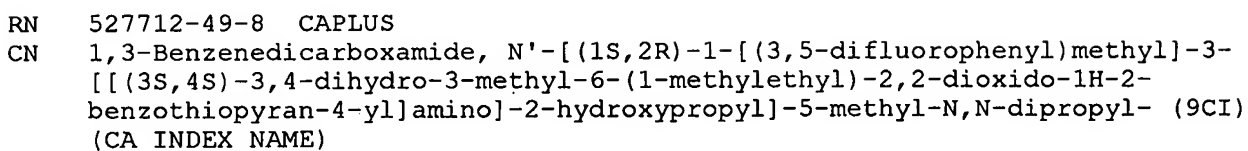
Absolute stereochemistry.



RN 527712-47-6 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3S,4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-3-propyl-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
(CA INDEX NAME)

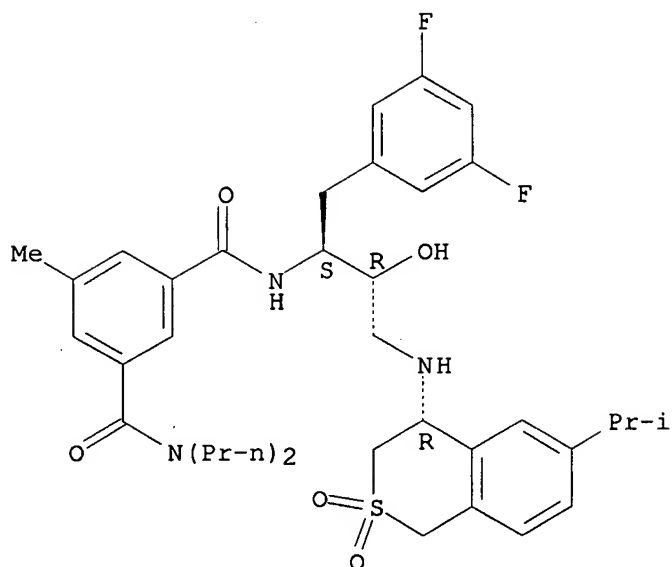
Absolute stereochemistry.



Chemical structure of a thienodibenzosulfone derivative. The structure features a central thienodibenzosulfone core. A 4-methyl-2-((n-propyl)2amino)benzoyl group is attached to the sulfur atom of the thiophene ring. A 2,4-difluorophenyl group is attached to the 2-position of the thiophene ring. A 1-(4-isopropylphenyl)ethan-1-yl group is attached to the 3-position of the thiophene ring. The stereochemistry is indicated with wedges and dashes.

RN	527712-51-2	CAPLUS
CN	1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI) (CA INDEX NAME)	

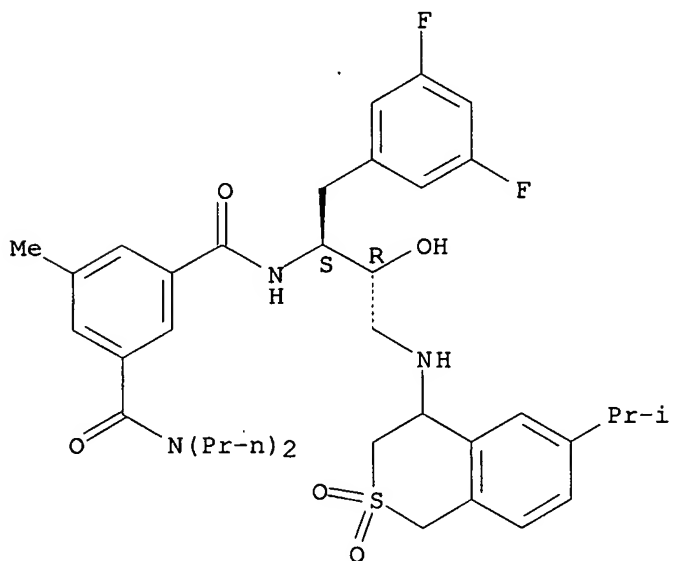
Absolute stereochemistry.



RN 527728-78-5 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI) (CA INDEX NAME)

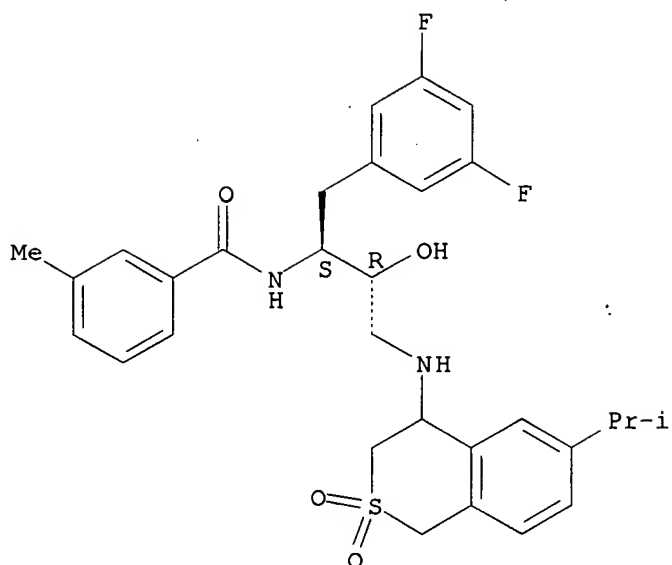
Absolute stereochemistry.



RN 527730-04-7 CAPLUS

CN Benamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-methyl- (9CI) (CA INDEX NAME)

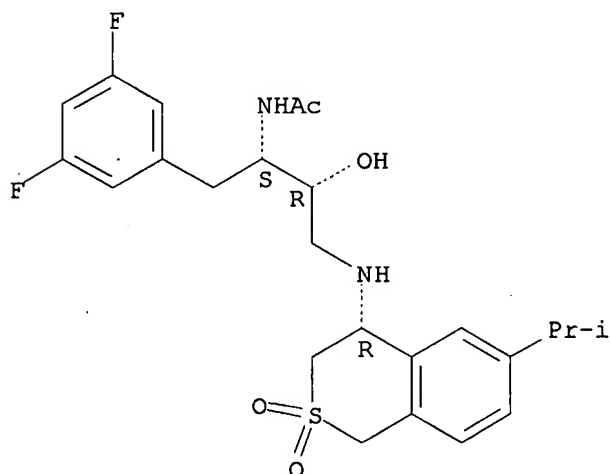
Absolute stereochemistry.



RN 527730-68-3 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[4R]-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

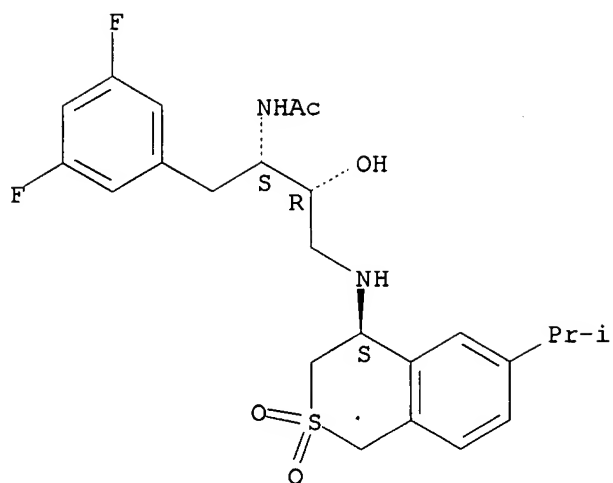
Absolute stereochemistry.



RN 527730-69-4 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[4S]-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

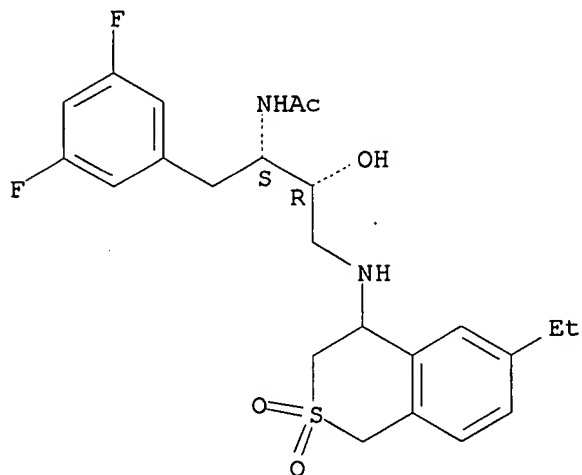
Absolute stereochemistry.



RN 527731-50-6 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-2-hydroxypropyl- (9CI) (CA INDEX NAME)

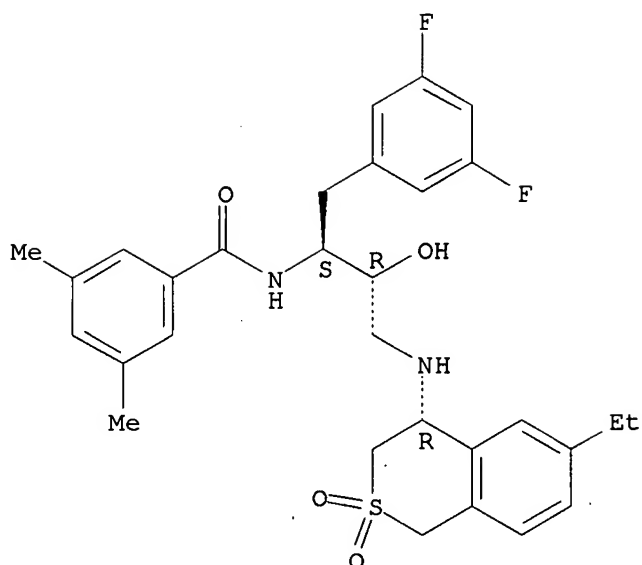
Absolute stereochemistry.



RN 527731-85-7 CAPLUS

CN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

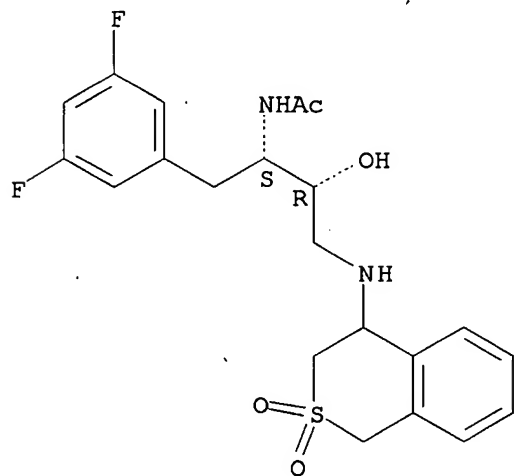
Absolute stereochemistry.



RN 527732-28-1 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

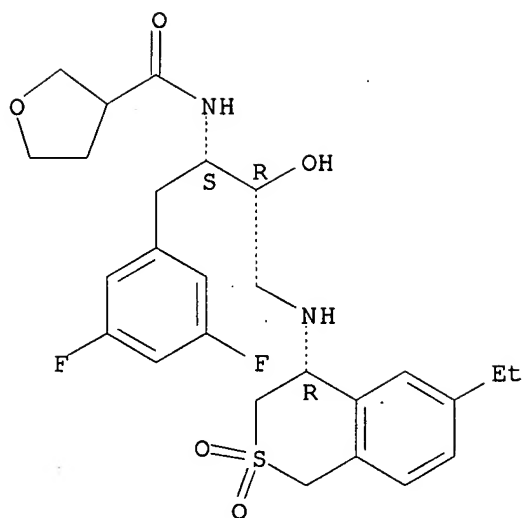
Absolute stereochemistry.



RN 527732-54-3 CAPLUS

CN 3-Furancarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]tetrahydro- (9CI) (CA INDEX NAME)

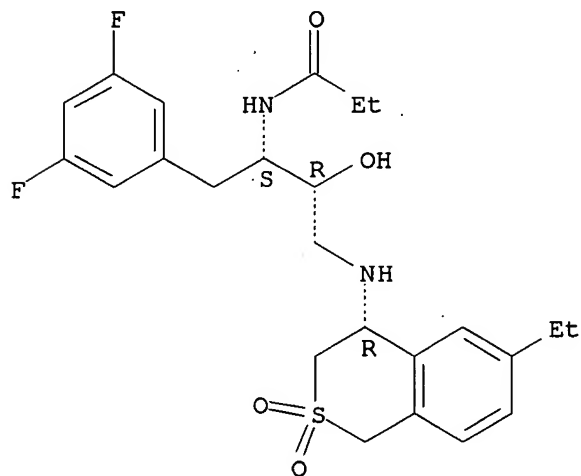
Absolute stereochemistry.



RN 527732-55-4 CAPLUS

CN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

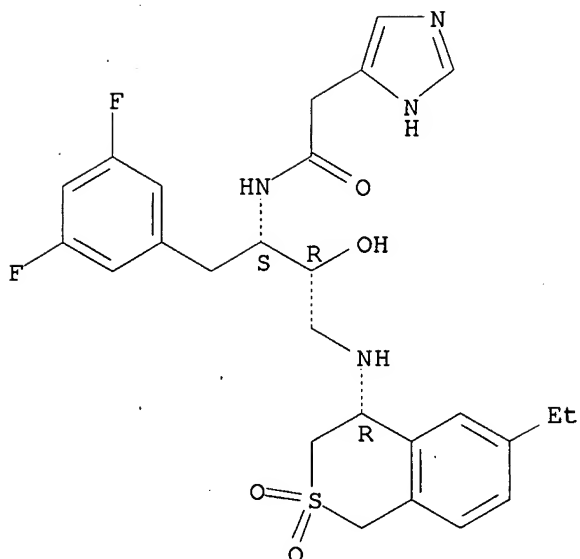
Absolute stereochemistry.



RN 527732-56-5 CAPLUS

CN 1H-Imidazole-4-acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

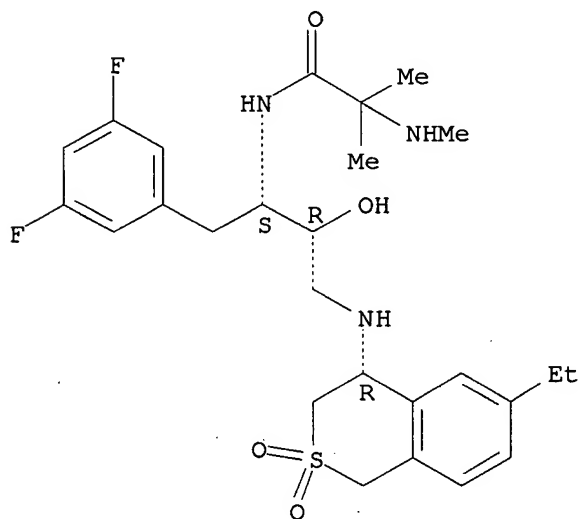
Absolute stereochemistry.



RN 527732-57-6 CAPLUS

CN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-2-methyl-2-(methylamino)- (9CI) (CA INDEX NAME)

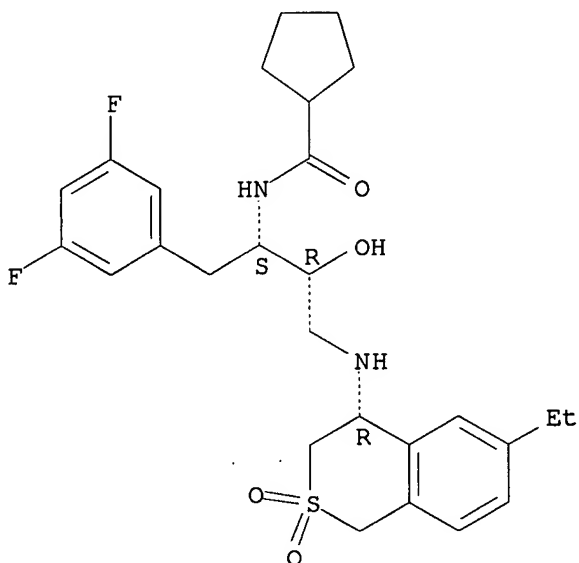
Absolute stereochemistry.



RN 527732-58-7 CAPLUS

CN Cyclopentanecarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

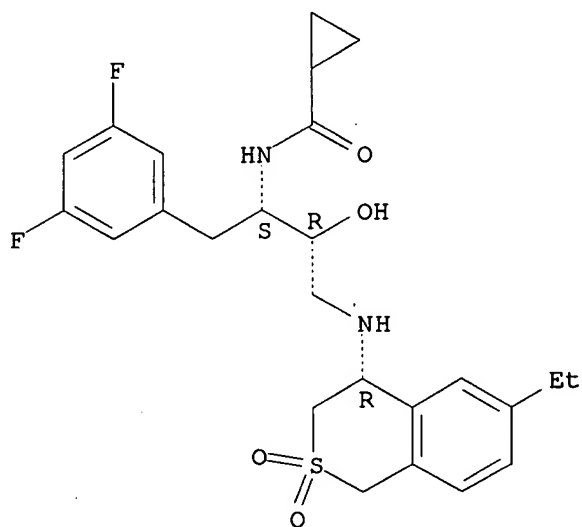
Absolute stereochemistry.



RN 527732-59-8 CAPLUS

CN Cyclopropanecarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

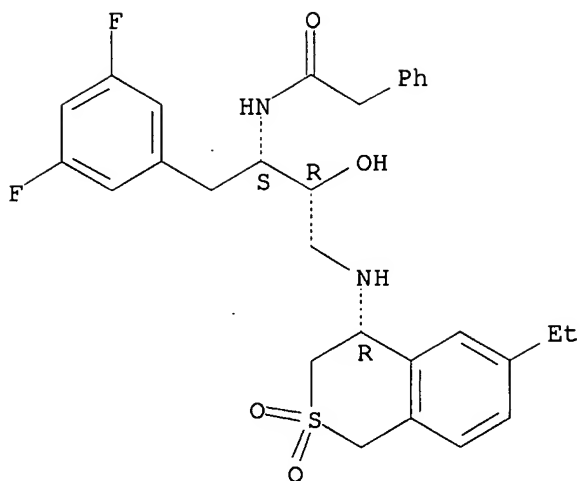
Absolute stereochemistry.



RN 527732-60-1 CAPLUS

CN Benzeneacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

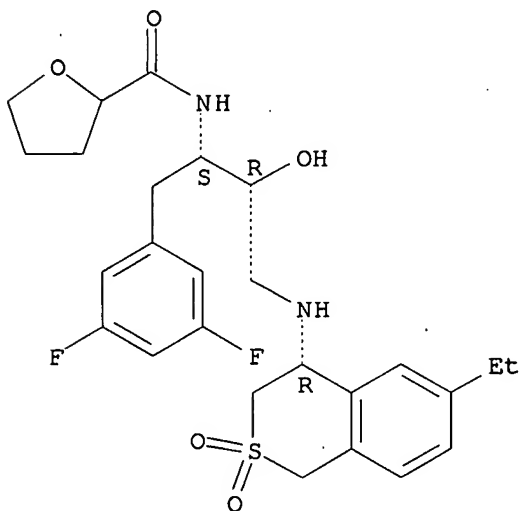
Absolute stereochemistry.



RN 527732-61-2 CAPLUS

CN 2-Furancarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]tetrahydro- (9CI) (CA INDEX NAME)

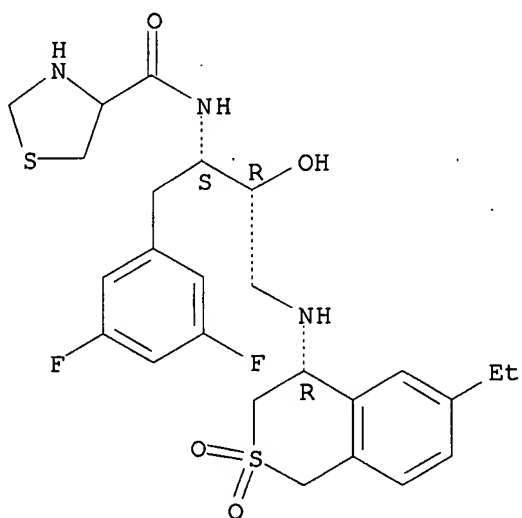
Absolute stereochemistry.



RN 527732-62-3 CAPLUS

CN 4-Thiazolidinecarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

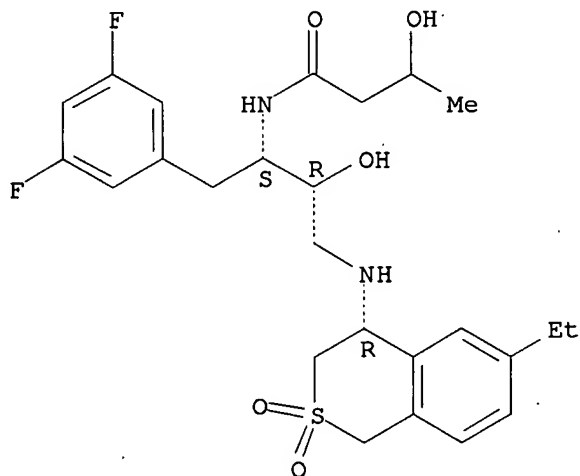
Absolute stereochemistry.



RN 527732-63-4 CAPLUS

CN Butanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-hydroxy- (9CI) (CA INDEX NAME)

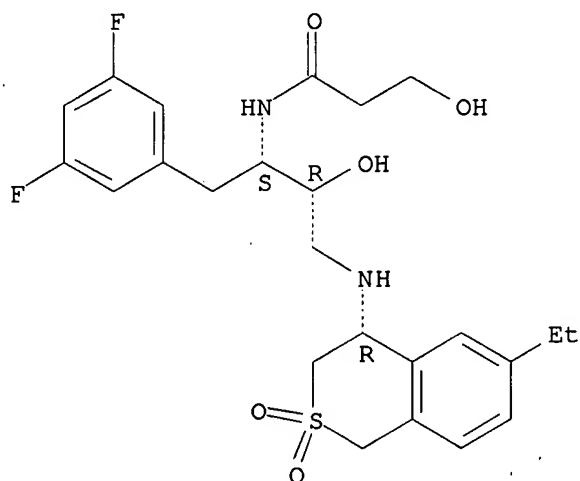
Absolute stereochemistry.



RN 527732-64-5 CAPLUS

CN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-hydroxy- (9CI) (CA INDEX NAME)

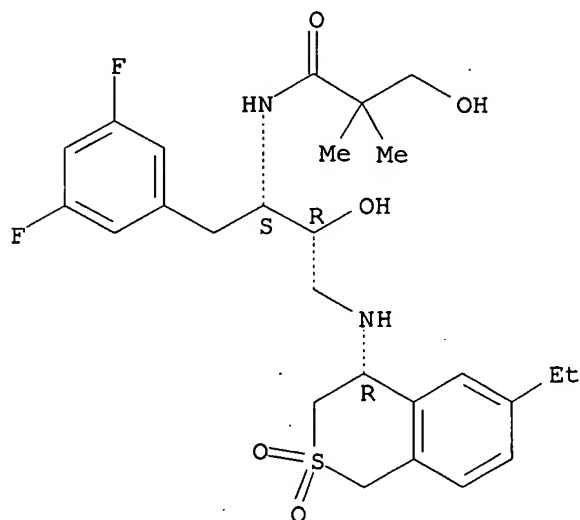
Absolute stereochemistry.



RN 527732-65-6 CAPLUS

CN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-hydroxy-2,2-dimethyl- (9CI) (CA INDEX NAME)

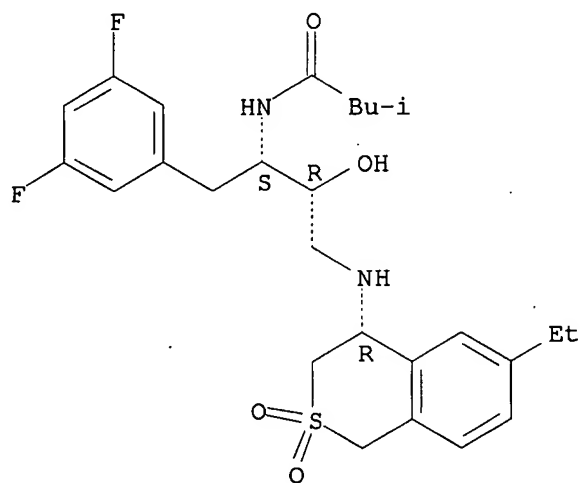
Absolute stereochemistry.



RN 527732-66-7 CAPLUS

CN Butanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-methyl- (9CI) (CA INDEX NAME)

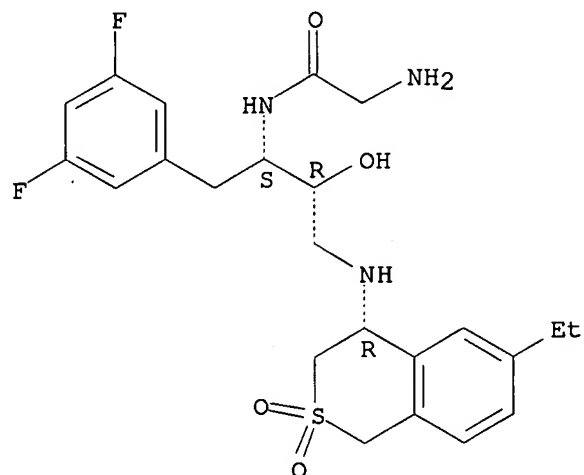
Absolute stereochemistry.



RN 527732-67-8 CAPLUS

CN Acetamide, 2-amino-N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

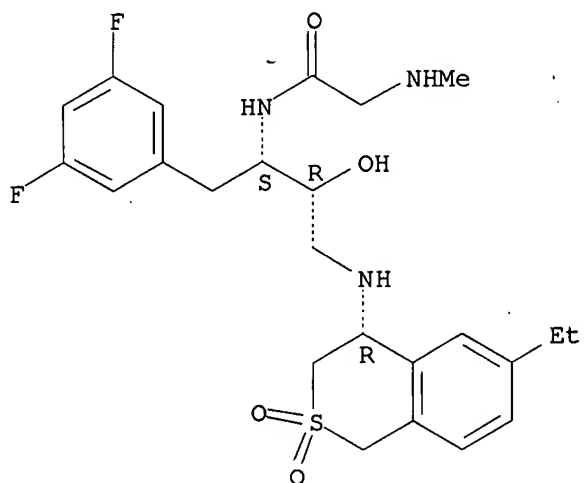
Absolute stereochemistry.



RN 527732-68-9 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-2-(methylamino)- (9CI) (CA INDEX NAME)

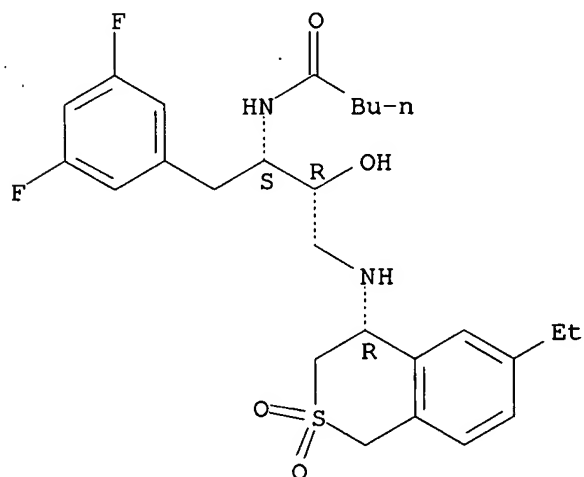
Absolute stereochemistry.



RN 527733-12-6 CAPLUS

CN Pentanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-(9CI) (CA INDEX NAME)

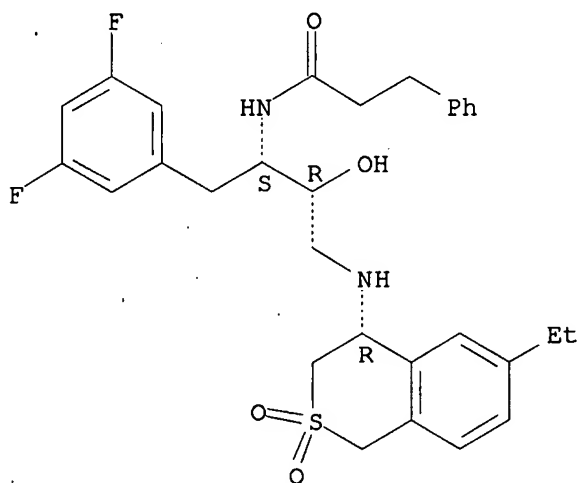
Absolute stereochemistry.



RN 527733-13-7 CAPLUS

CN Benzenepropanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-(9CI) (CA INDEX NAME)

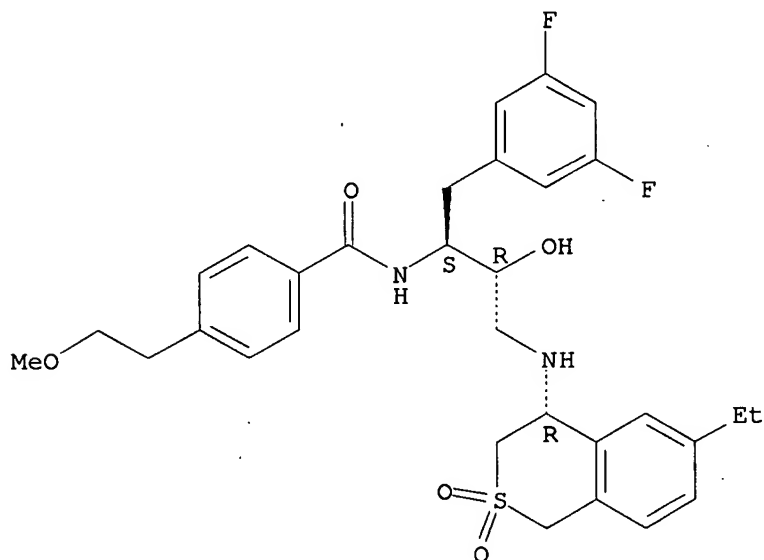
Absolute stereochemistry.



RN 527733-19-3 CAPLUS

CN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-4-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

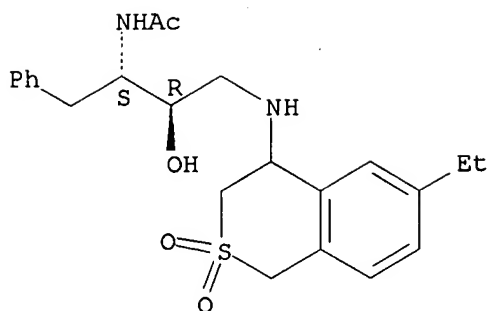
Absolute stereochemistry.



RN 527733-26-2 CAPLUS

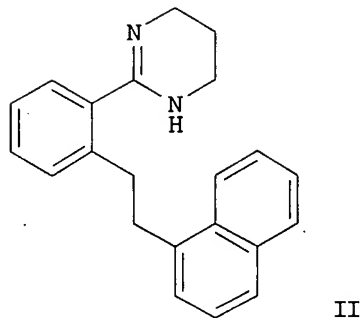
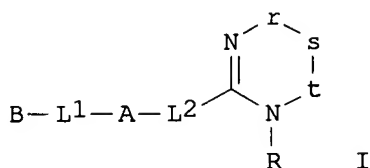
CN Acetamide, N-[(1S,2R)-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxy-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2002:615577 CAPLUS
 DN 137:169536
 TI Preparation of aryl-substituted tetrahydropyrimidines and related
 compounds as melanocortin-4 receptor binding compounds
 IN Maguire, Martin P.; Dai, Mingshi; Vos, Tricia J.
 PA Millennium Pharmaceuticals, Inc., USA
 SO PCT Int. Appl., 228 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002062766	A2	20020815	WO 2002-US3566	20020207
	WO 2002062766	A3	20021003		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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	US 2000-223277P	P	20000803		
	US 2000-632309	A2	20000804		
	WO 2002-US3566	W	20020207		
OS	MARPAT 137:169536				
GI					



AB Title compds. I [wherein A and B = independently (un)substituted biaryl, (hetero)aryl, Ph, (cyclo)alkyl, (cyclo)alkoxy, alkenyl, alkynyl, OH, acyl(oxy), carbamoyl, amino, thiol, amidino, imino, NO₂, N₃, etc.; L₁ and L₂ = covalent bond or (un)substituted alkyl optionally interrupted by O, S, or N; r = covalent bond, CH, CH₂, CHR₁, CR₁R₂, or H; t = CH, CH₂, CHR₃, CR₃R₄, or H; s = CHR₅, CR₅R₆, or absent; R = H, (un)substituted alkyl, arylalkyl, or heteroalkyl, and may optionally be linked to A, B, L₁, or L₂; R₁-R₆ = independently (un)substituted alkyl, halo, thiol, thioether, thioalkyl, alkoxy, and may be optionally linked to each other to form addnl. ring moieties, e.g., quinoxaliny; or pharmaceutically acceptable salts thereof] were prepared as melanocortin-4 receptor binding (MC4-R) compds. For example, stirring a solution of α -tolunitrile with diisopropylamine and BuLi in hexanes at -78° under nitrogen for 1 h, followed by addition of HMPA and 1-chloromethylnaphthalene in THF, afforded 2-(2-naphthalen-1-ylethyl)benzonitrile. Heating the benzonitrile with 1,3-diaminopropane in the presence of H₂S at 80° for 72 h gave the tetrahydropyrimidinyl cycloaddn. product II. The latter exhibited exemplary inhibition of MC4-R in a scintillation proximity assay. I are useful for the treatment of disorders associated with pigmentation, bones, or weight loss (no data).

IT 447462-54-6P, 1-Amino-3-[2-(5-bromo-2-methoxyphenyl)-7-chlorobenzo[b]thiophen-3-ylamino]propan-2-ol 447462-69-3P, 1-Amino-3-[2-(5-bromo-2-methoxyphenyl)-7-fluorobenzo[b]thiophen-3-ylamino]propan-2-ol

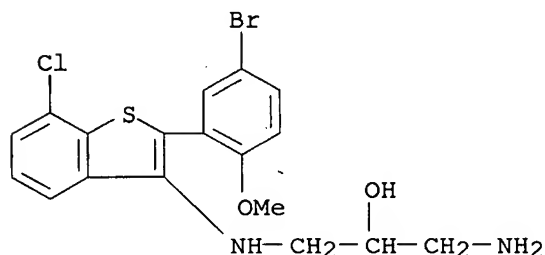
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(MC4-R binding compound; preparation of aryl-substituted tetrahydropyrimidines

and related compds. as melanocortin-4 receptor binding compds. for treatment of pigmentation, bone, and weight loss disorders)

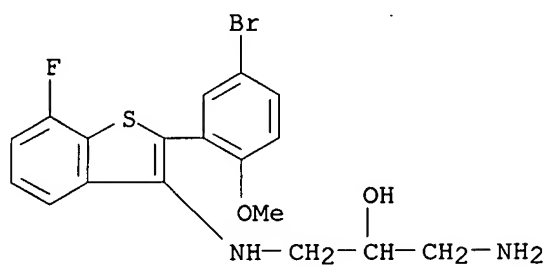
RN 447462-54-6 CAPLUS

CN 2-Propanol, 1-amino-3-[[2-(5-bromo-2-methoxyphenyl)-7-chlorobenzo[b]thien-3-yl]amino]- (9CI) (CA INDEX NAME)



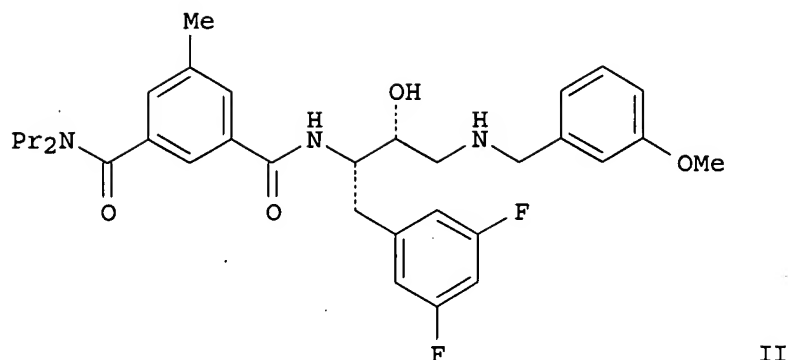
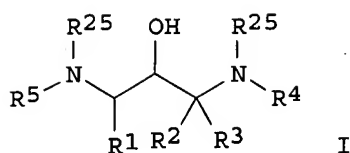
RN 447462-69-3 CAPLUS

CN 2-Propanol, 1-amino-3-[[2-(5-bromo-2-methoxyphenyl)-7-fluorobenzo[b]thien-3-yl]amino]- (9CI) (CA INDEX NAME)



AN 2003:376819 CAPLUS
 DN 138:385173
 TI Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease
 IN Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy
 PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
 SO PCT Int. Appl., 1243 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 2

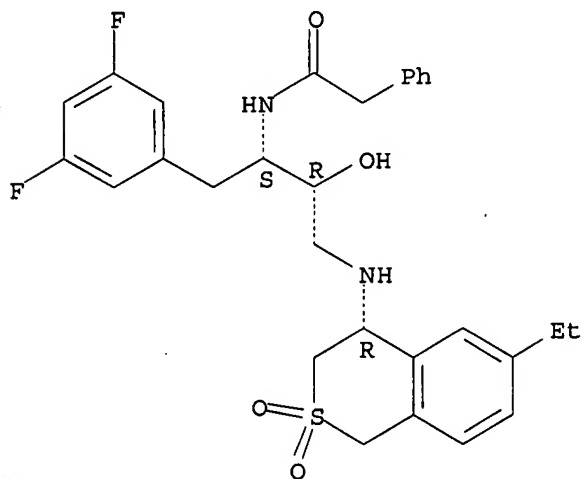
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PI	WO 2003040096	A2	20030515	WO 2002-US36072	20021108
	WO 2003040096	A3	20040506		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
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	WO 2003040096	A2	20030515	WO 2002-XA36072	20021108
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	AU 2002359376	A1	20030519	AU 2002-359376	20021108
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	JP 2005520791	T	20050714	JP 2003-542142	20021108
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	NZ 533107	A	20070427	NZ 2002-533107	20021108
	ZA 2004003578	A	20051010	ZA 2004-3578	20040511
	IN 2004KN00627	A	20060224	IN 2004-KN627	20040514
	NO 2004002359	A	20040806	NO 2004-2359	20040607
PRAI	US 2001-337122P	P	20011108		
	US 2001-344086P	P	20011228		
	US 2002-345635P	P	20020103		
	WO 2002-US36072	W	20021108		
OS	MARPAT 138:385173				
GI					



AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, etc.; or R2 and R3 are taken together with the carbon to which they are attached to form a carbocycle of 3-7 carbon atoms, optionally where one carbon atom is replaced by a heteroatom selected from the group consisting of O, S, SO₂, (un)substituted NH; R4 = alkyl, haloalkyl, hydroxyalkyl, etc.; R5 = R6X (wherein X = CO, SO₂, (un)substituted CH₂; R6 = (un)substituted Ph, naphthyl, indanyl, etc.); R25 = H, alkyl, alkoxy, etc.] which have activity as inhibitors of β -secretase and are therefore useful in treating a variety of disorders such as Alzheimer's disease, were prepared E.g., a multi-step synthesis of (1S,2R)-II, starting from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic acid, was given. The compds. I showed IC₅₀ of < 20 μ M in cell free inhibition assay utilizing a synthetic APP substrate. This is a Part 1 of 1-2 series.

RN 527732-60-1 REGISTRY
 ED Entered STN: 09 Jun 2003
 CN Benzeneacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C29 H32 F2 N2 O4 S
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.

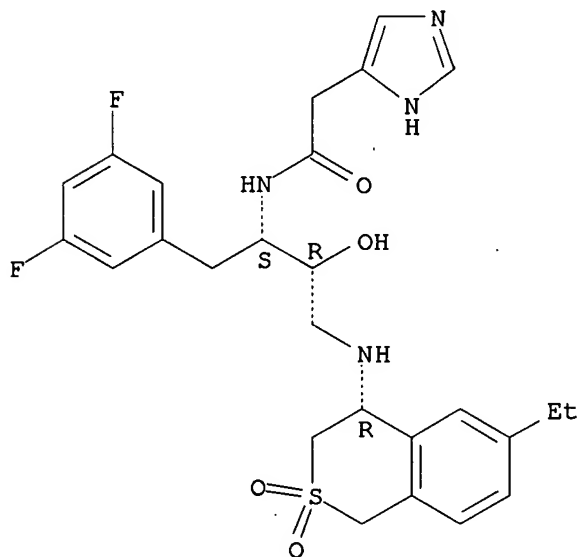


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 527732-56-5 REGISTRY
 ED Entered STN: 09 Jun 2003
 CN 1H-Imidazole-4-acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-
 [[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
 hydroxypropyl]- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C26 H30 F2 N4 O4 S
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

Absolute stereochemistry.



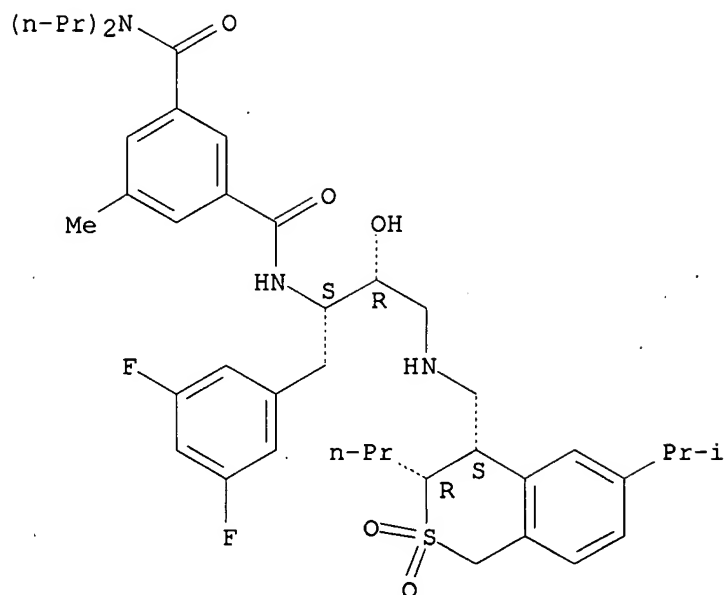
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d scan 17

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
 3-[[[(3R,4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-3-propyl-1H-2-
 benzothiopyran-4-yl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-
 (9CI)
 MF C41 H55 F2 N3 O5 S

Absolute stereochemistry.

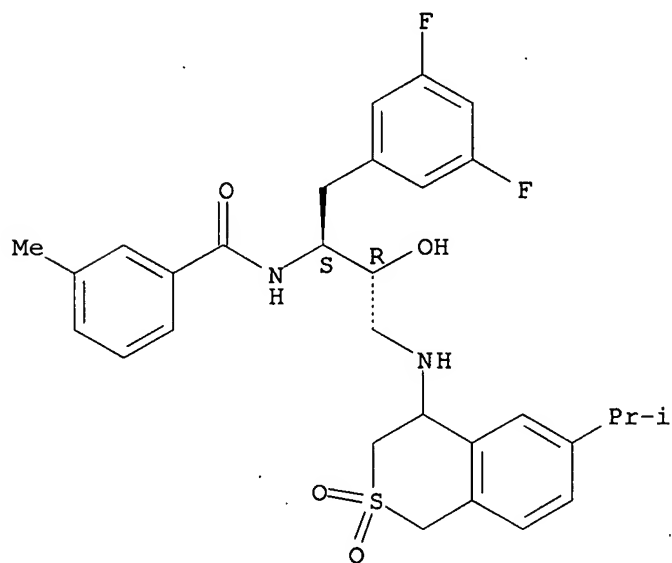


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):43

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[3,4-dihydro-
 6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
 hydroxypropyl]-3-methyl- (9CI)
 MF C30 H34 F2 N2 O4 S

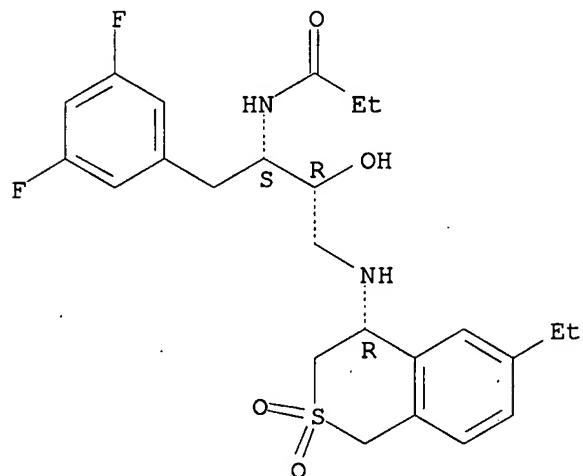
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI)
 MF C24 H30 F2 N2 O4 S

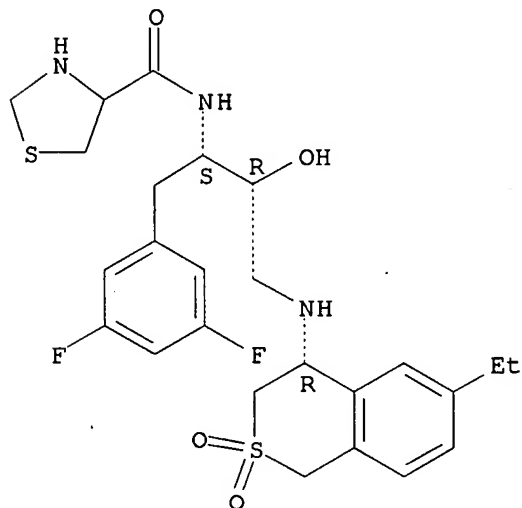
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 4-Thiazolidinecarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI)
 MF C25 H31 F2 N3 O4 S2

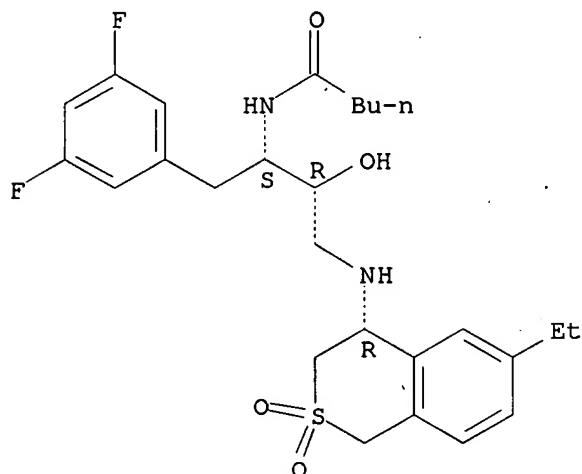
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Pentanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI)
MF C26 H34 F2 N2 O4 S

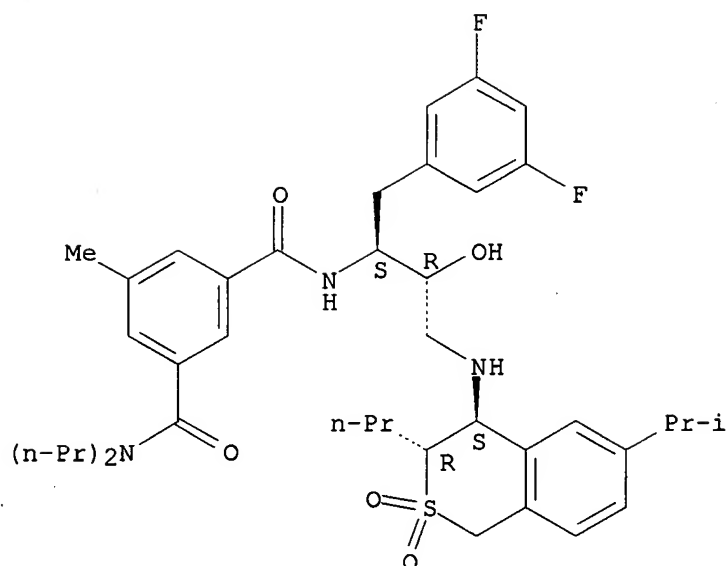
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3R,4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-3-propyl-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
MF C40 H53 F2 N3 O5 S

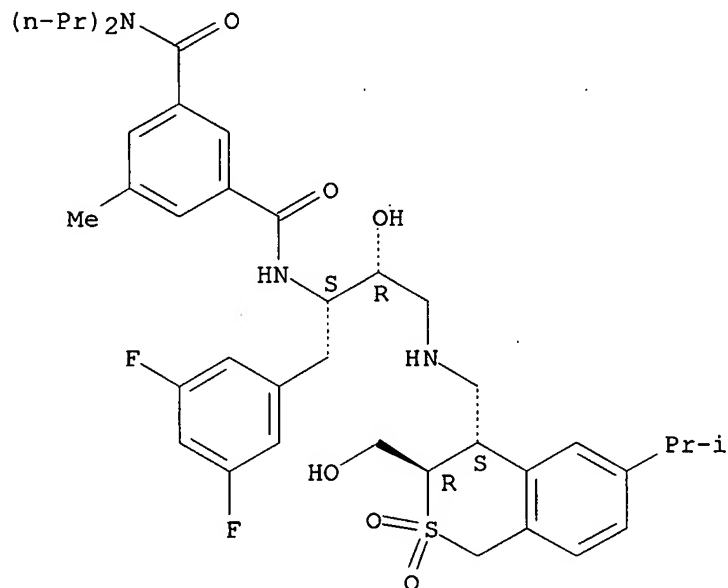
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3R,4S)-3,4-dihydro-3-(hydroxymethyl)-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
 MF C39 H51 F2 N3 O6 S

Absolute stereochemistry.

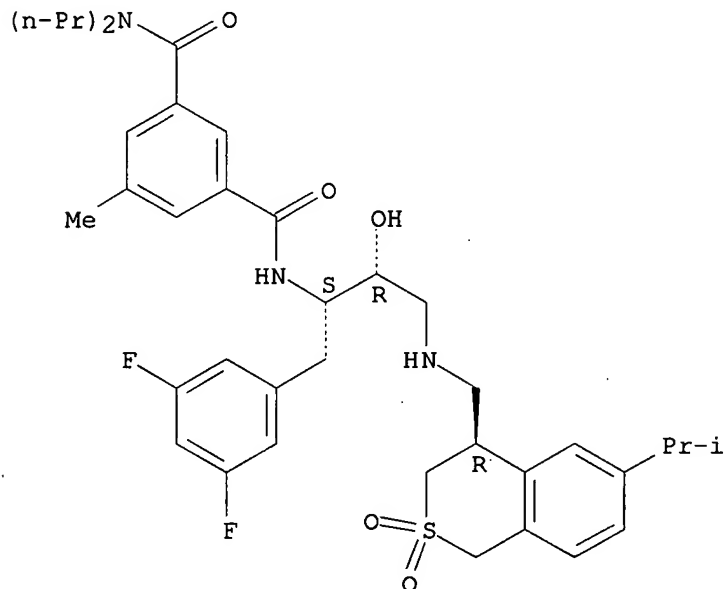


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
3-[[[(4R)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-
yl)methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
MF C38 H49 F2 N3 O5 S

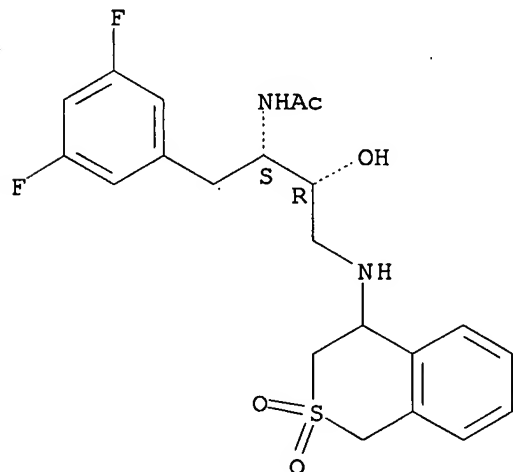
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(3,4-dihydro-
2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]- (9CI)
MF C21 H24 F2 N2 O4 S

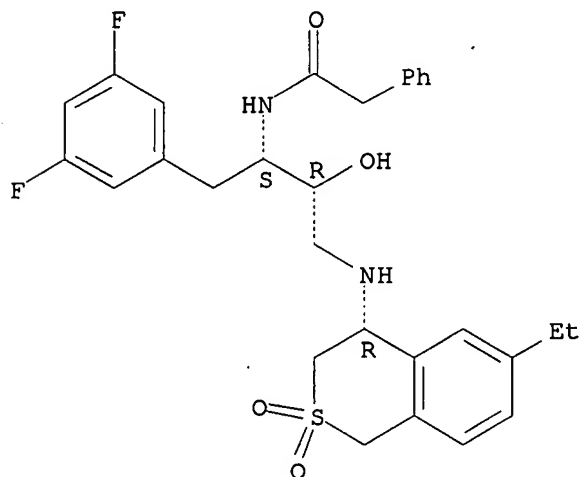
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzeneacetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-
6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
hydroxypropyl]- (9CI)
MF C29 H32 F2 N2 O4 S

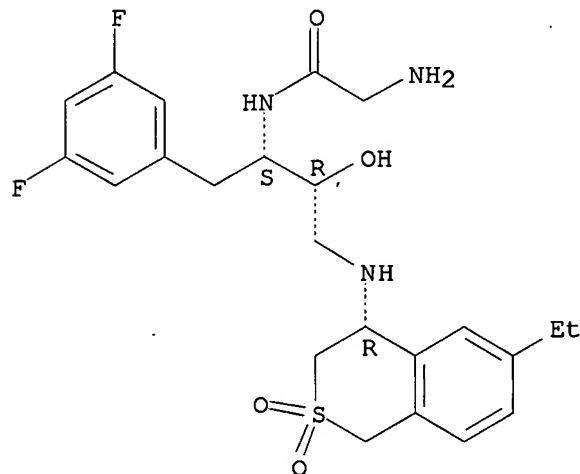
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Acetamide, 2-amino-N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-
6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
hydroxypropyl]- (9CI)
MF C23 H29 F2 N3 O4 S

Absolute stereochemistry.



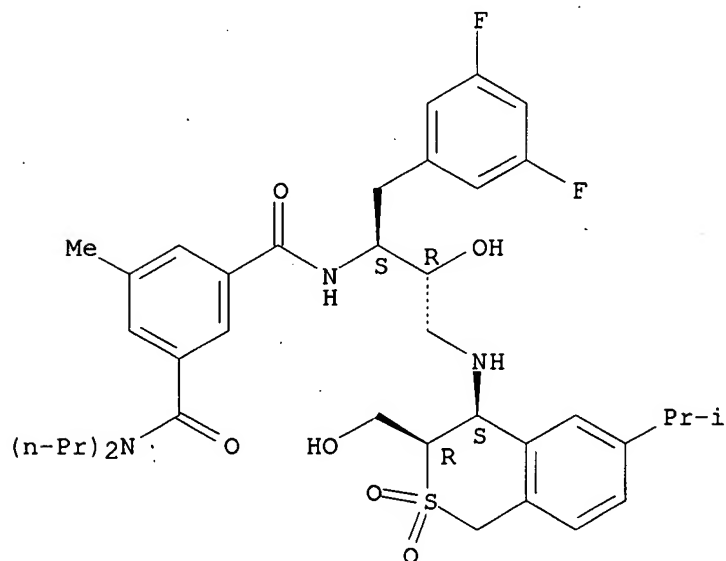
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3R,4S)-3,4-dihydro-3-(hydroxymethyl)-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-(9CI)

MF C38 H49 F2 N3 O6 S

Absolute stereochemistry.



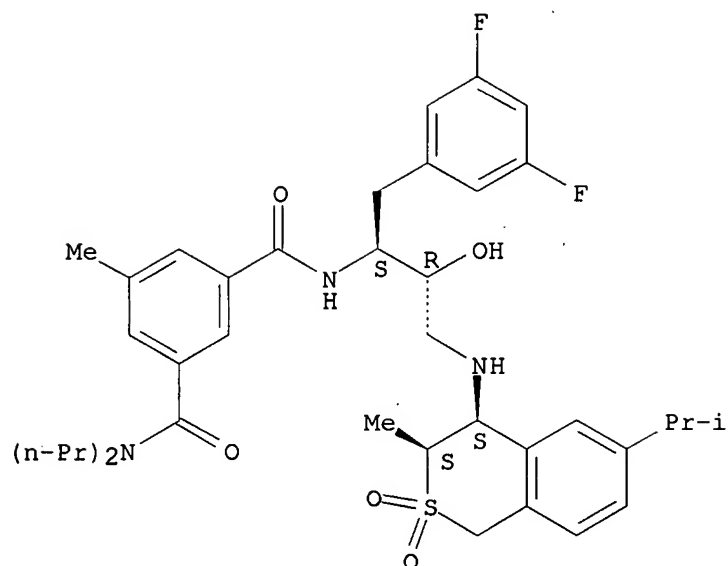
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3S,4S)-3,4-dihydro-3-methyl-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-(9CI)

MF C38 H49 F2 N3 O5 S

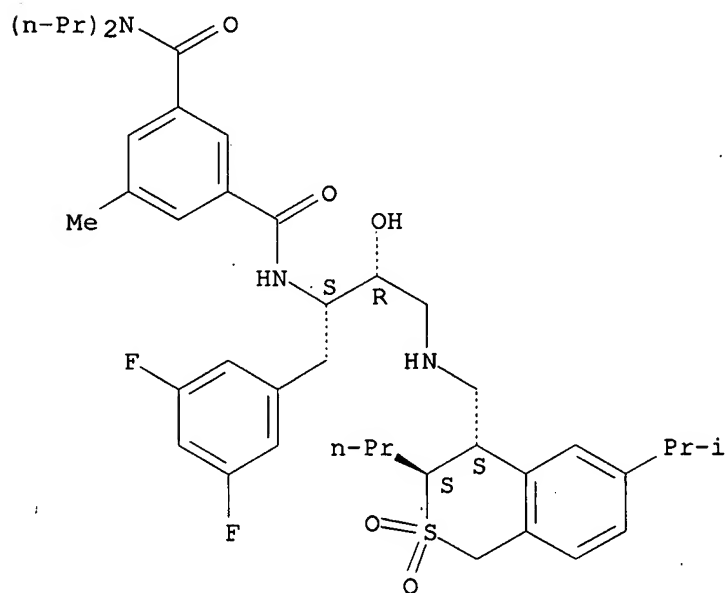
Absolute stereochemistry.



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
 3-[[[(3S,4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-3-propyl-1H-2-
 benzothiopyran-4-yl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-
 (9CI)
 MF C41 H55 F2 N3 O5 S

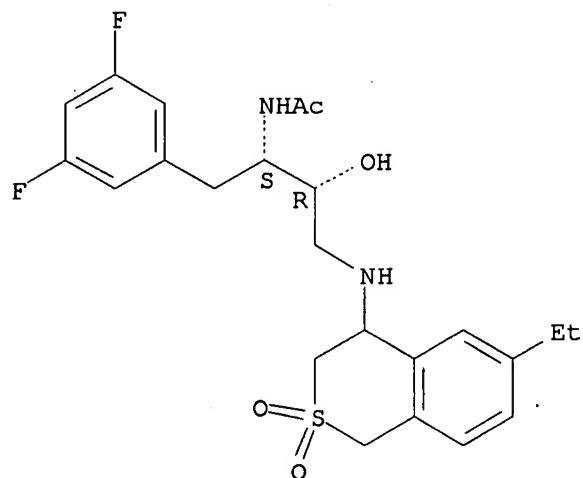
Absolute stereochemistry.



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxypropyl]-
 (9CI)
 MF C23 H28 F2 N2 O4 S

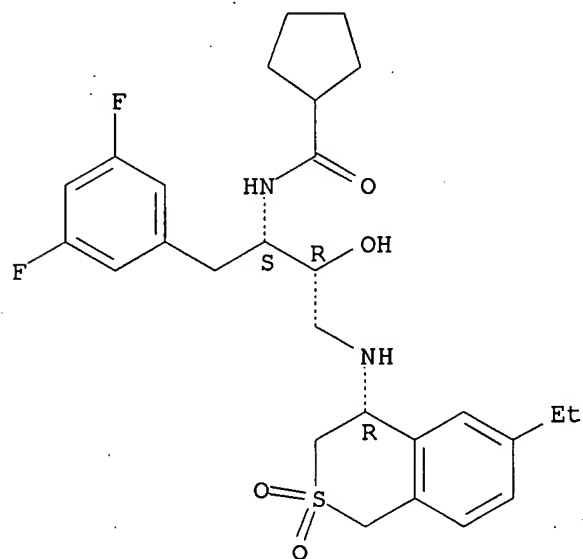
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Cyclopentanecarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-
 [[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
 hydroxypropyl]- (9CI)
 MF C27 H34 F2 N2 O4 S

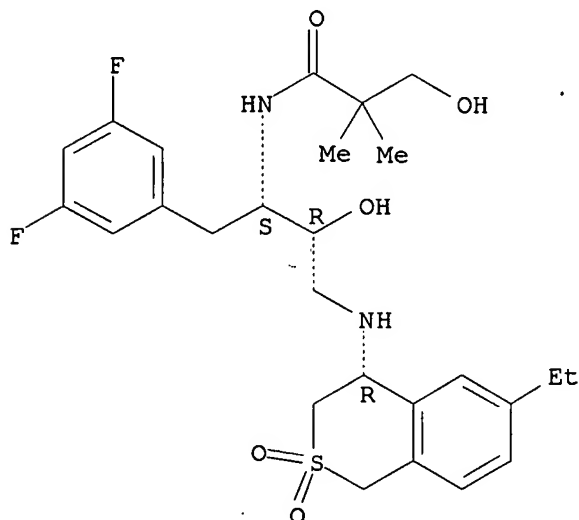
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-hydroxy-2,2-dimethyl- (9CI)
MF C26 H34 F2 N2 O5 S

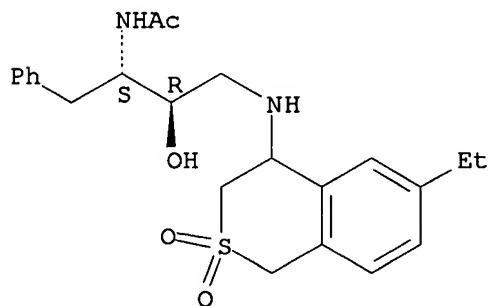
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Acetamide, N-[(1S,2R)-3-[(6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl)amino]-2-hydroxy-1-(phenylmethyl)propyl]- (9CI)
MF C23 H30 N2 O4 S

Absolute stereochemistry.



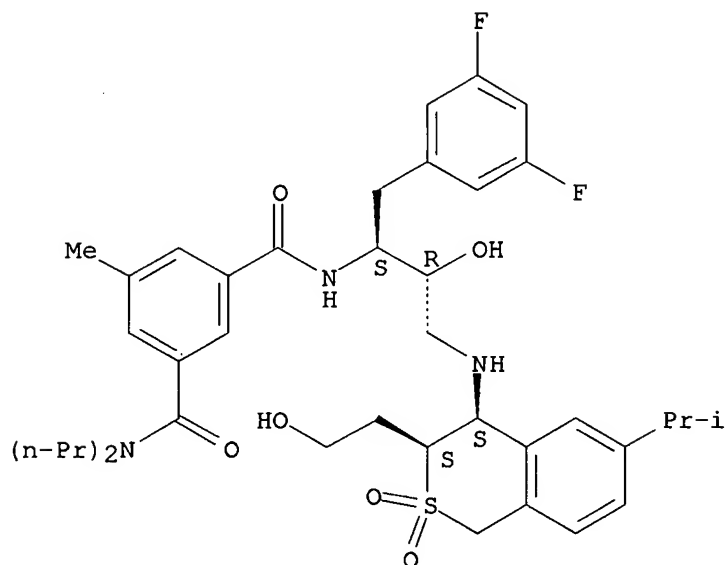
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3S,4S)-3,4-dihydro-3-(2-hydroxyethyl)-6-(1-methylethyl)-2,2-dioxido-

1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-
(9CI)

MF C39 H51 F2 N3 O6 S

Absolute stereochemistry.



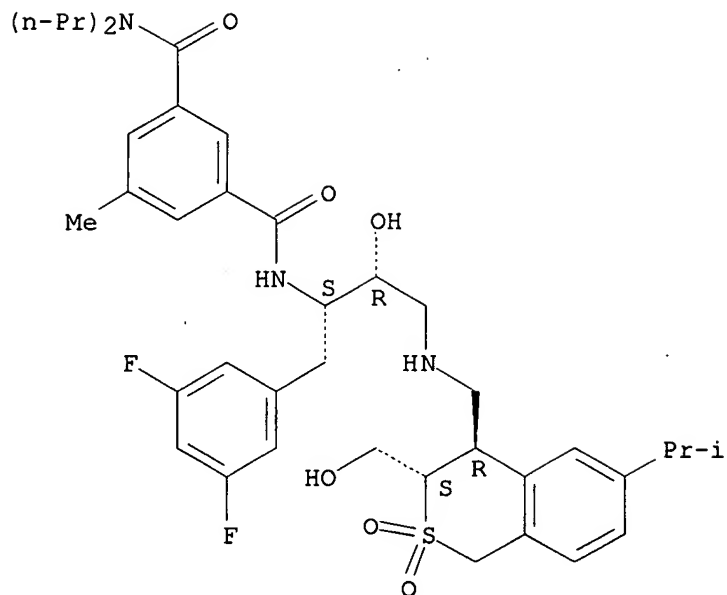
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
3-[[[(3S,4R)-3,4-dihydro-3-(hydroxymethyl)-6-(1-methylethyl)-2,2-dioxido-
1H-2-benzothiopyran-4-yl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-
dipropyl- (9CI)

MF C39 H51 F2 N3 O6 S

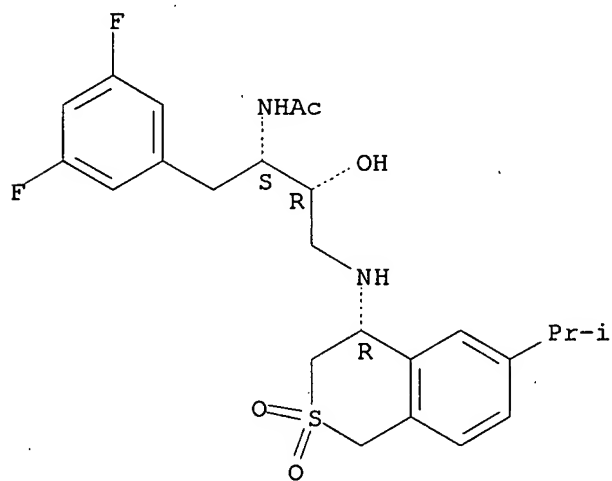
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI)
 MF C24 H30 F2 N2 O4 S

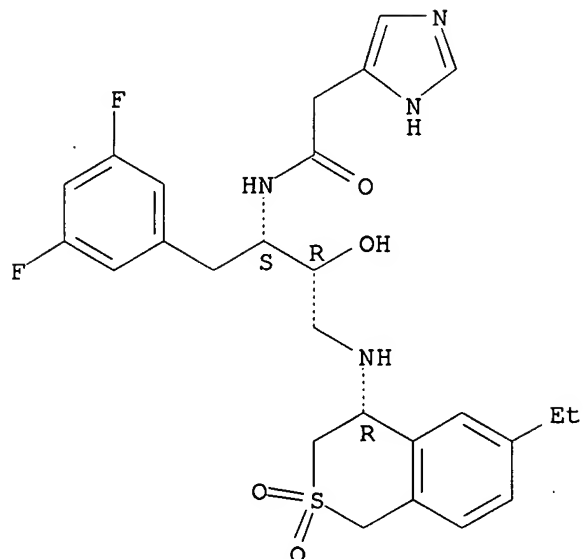
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1H-Imidazole-4-acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI)
 MF C26 H30 F2 N4 O4 S

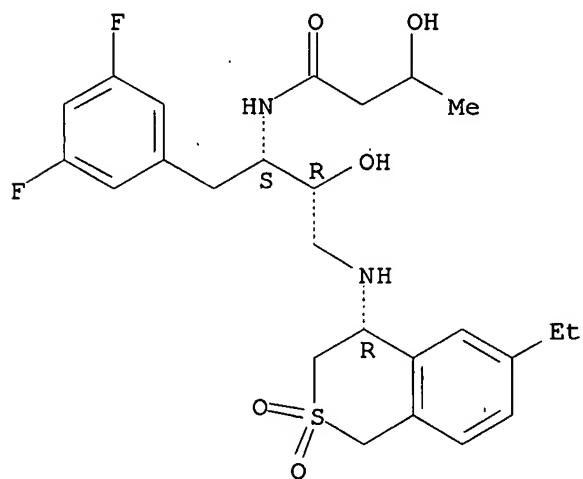
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Butanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-hydroxy- (9CI)
 MF C25 H32 F2 N2 O5 S

Absolute stereochemistry.

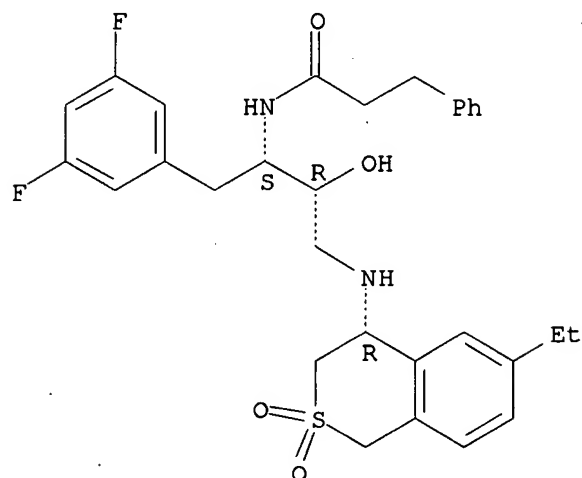


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Benzenepropanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-

hydroxypropyl]- (9CI)
MF C30 H34 F2 N2 O4 S

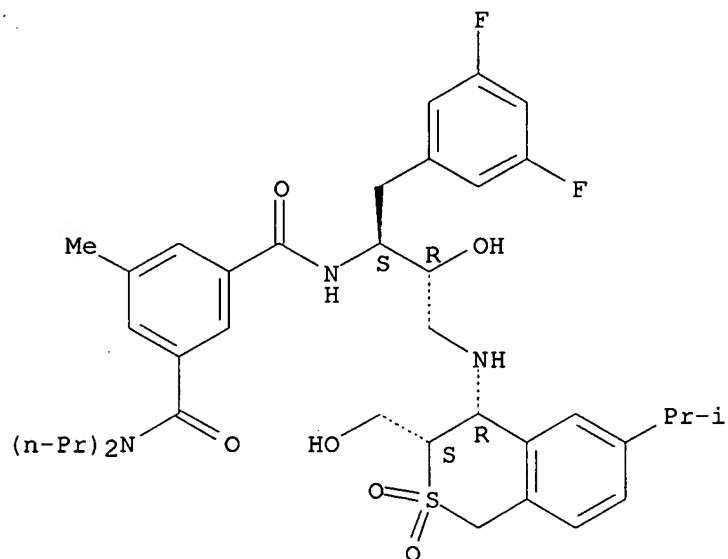
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
3-[[[(3S,4R)-3,4-dihydro-3-(hydroxymethyl)-6-(1-methylethyl)-2,2-dioxido-1H-
2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-
(9CI)
MF C38 H49 F2 N3 O6 S

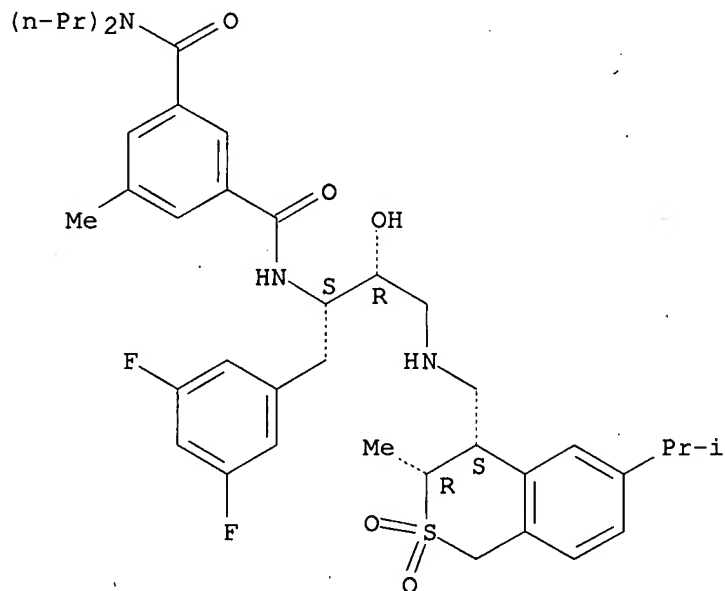
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
3-[[[(3R,4S)-3,4-dihydro-3-methyl-6-(1-methylethyl)-2,2-dioxido-1H-2-
benzothiopyran-4-yl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-
(9CI)
MF C39 H51 F2 N3 O5 S

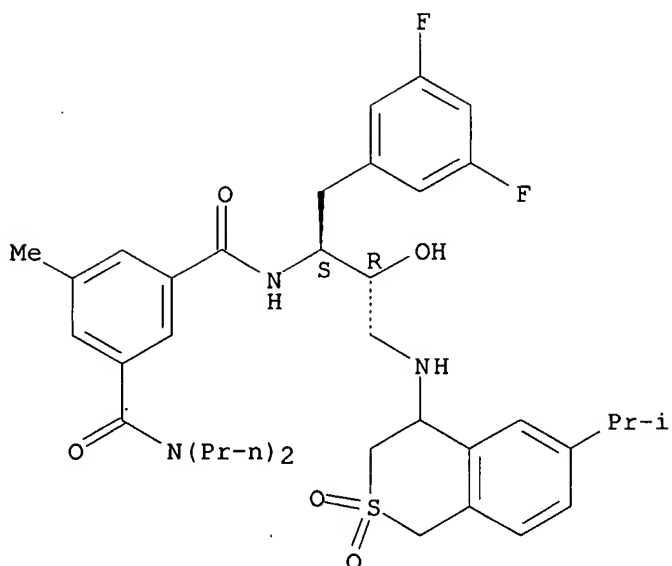
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
3-[[3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-
yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
MF C37 H47 F2 N3 O5 S

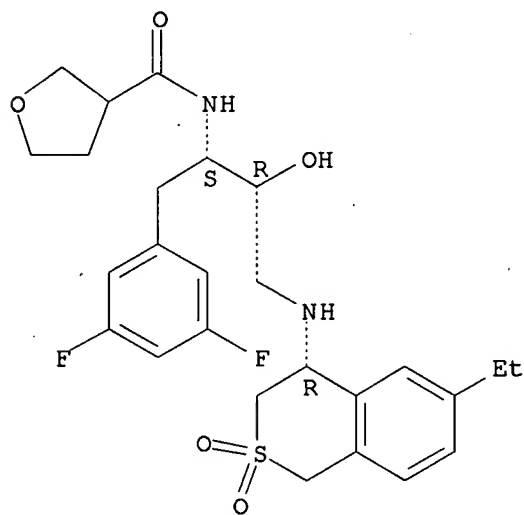
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 3-Furancarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-
 [[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
 hydroxypropyl]tetrahydro- (9CI)
 MF C26 H32 F2 N2 O5 S

Absolute stereochemistry.

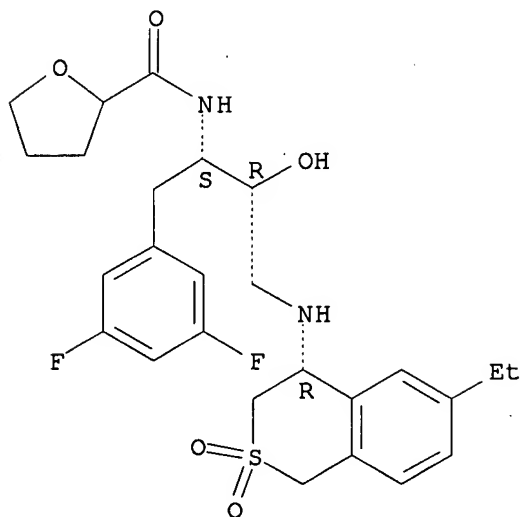


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 2-Furancarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-
 [[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
 hydroxypropyl]tetrahydro- (9CI)

MF C26 H32 F2 N2 O5 S

Absolute stereochemistry.



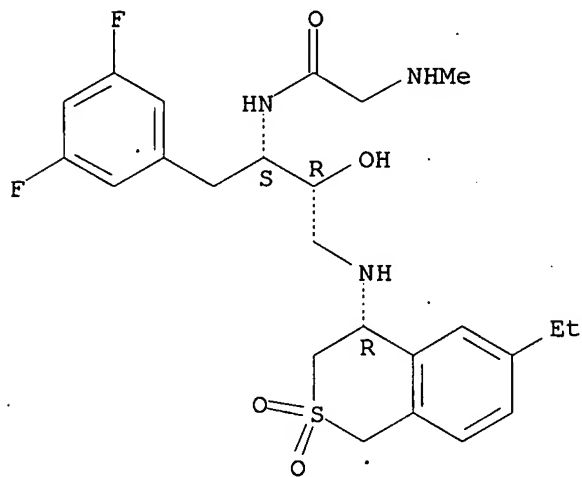
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Acetamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[4R)-6-ethyl-3,4-dihydro-2,2-dioxo-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-2-(methylamino)- (9CI)

MF C24 H31 F2 N3 O4 S

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

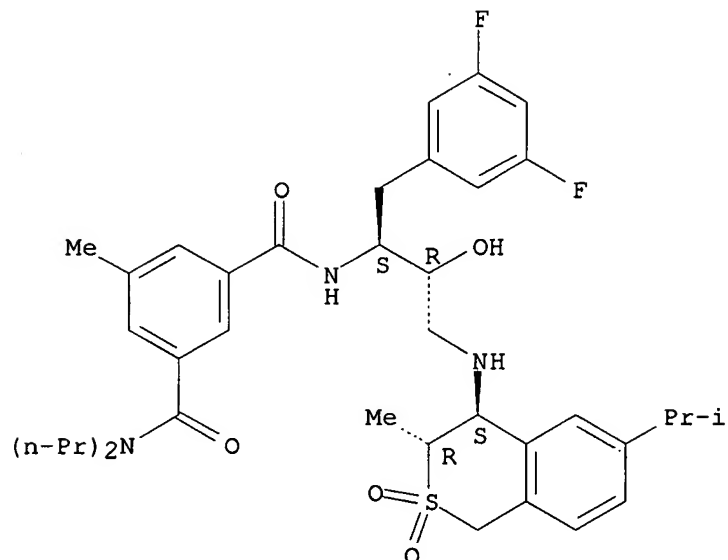
L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[3R,4S)-3-methyl-6-(1-methylethyl)-2,2-dioxo-1H-2-

benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-
(9CI)

MF C38 H49 F2 N3 O5 S

Absolute stereochemistry.



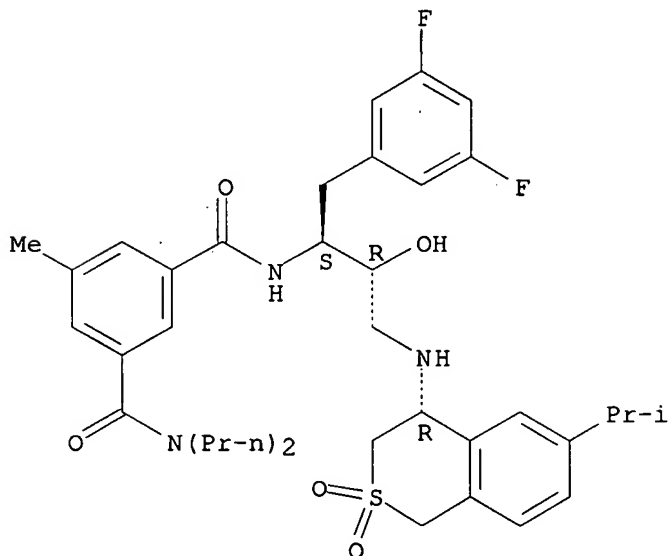
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
3-[[(4R)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-
yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)

MF C37 H47 F2 N3 O5 S

Absolute stereochemistry.



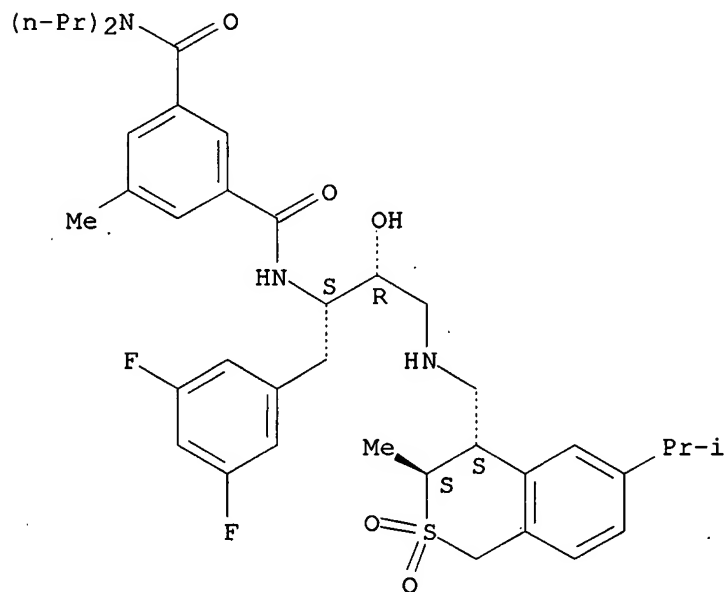
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(3S,4S)-3,4-dihydro-3-methyl-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-(9CI)

MF C39 H51 F2 N3 O5 S

Absolute stereochemistry.



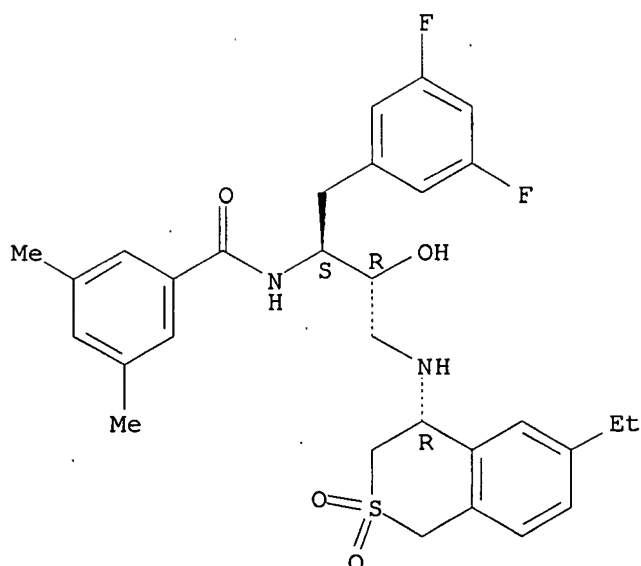
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3,5-dimethyl-(9CI)

MF C30 H34 F2 N2 O4 S

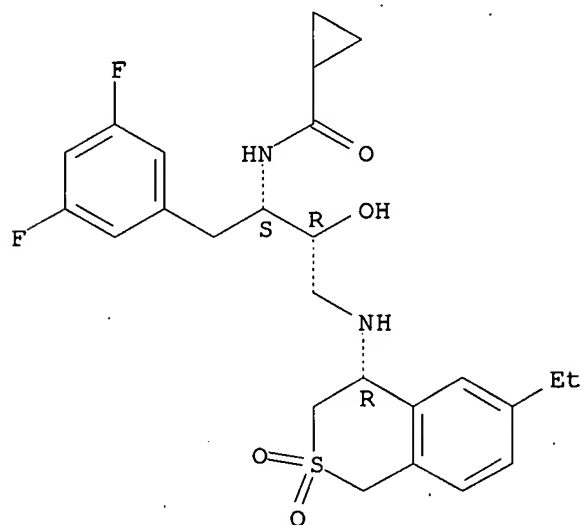
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Cyclopropanecarboxamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-
 [[(4R)-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
 hydroxypropyl]- (9CI)
 MF C25 H30 F2 N2 O4 S

Absolute stereochemistry.

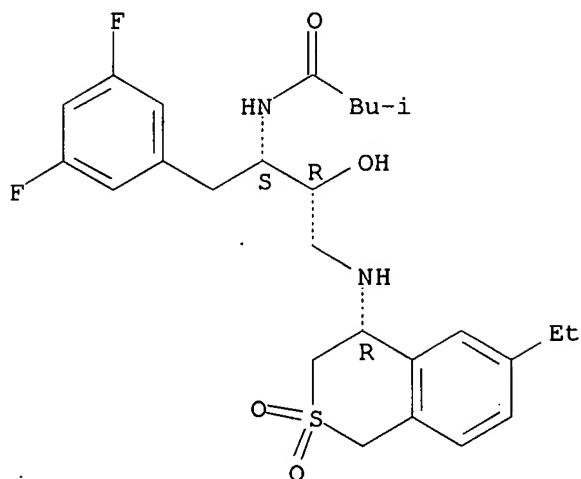


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Butanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(4R)-6-
 ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-
 hydroxypropyl]-3-methyl- (9CI)

MF C26 H34 F2 N2 O4 S

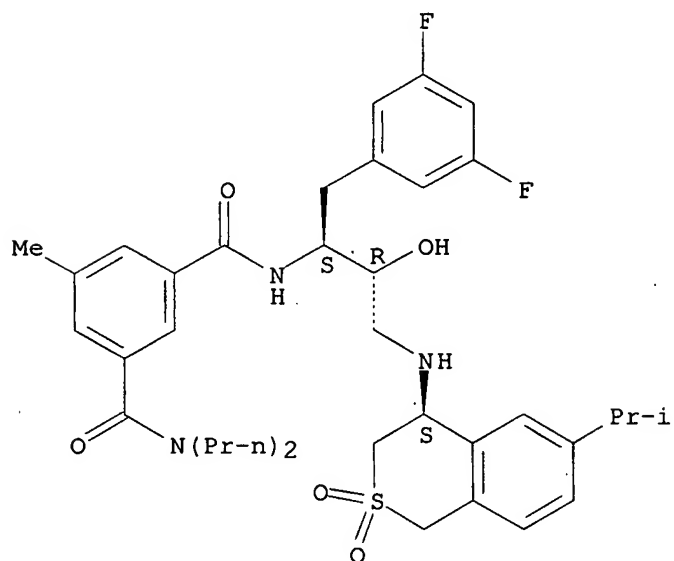
. Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
3-[[[(4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-
yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI)
MF C37 H47 F2 N3 O5 S

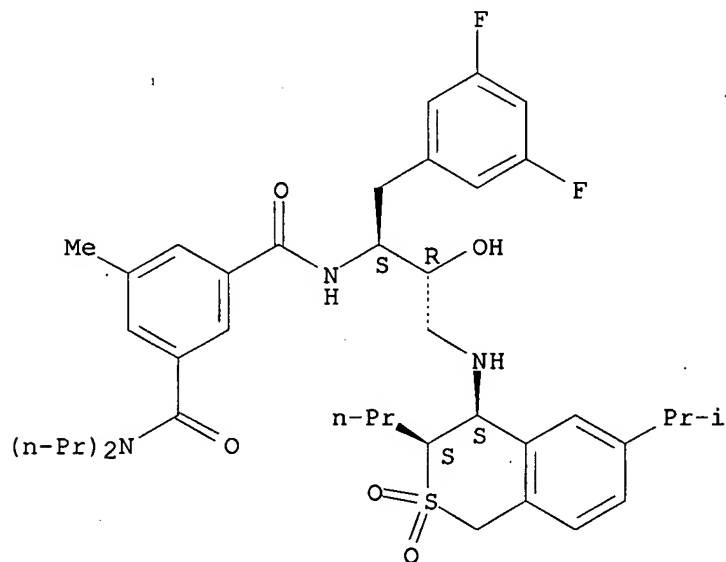
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
 3-[[(3S,4S)-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-3-propyl-1H-2-
 benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-
 (9CI)
 MF C40 H53 F2 N3 O5 S

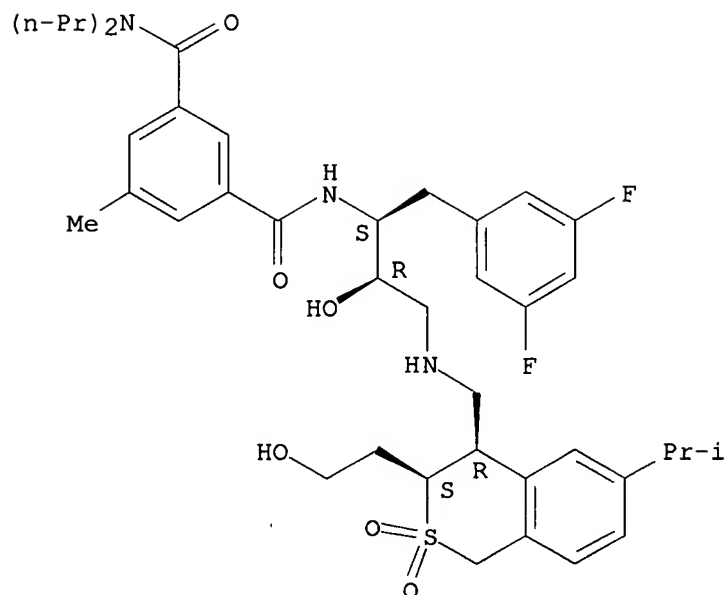
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
 3-[[[(3S,4R)-3,4-dihydro-3-(2-hydroxyethyl)-6-(1-methylethyl)-2,2-dioxido-
 1H-2-benzothiopyran-4-yl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-
 dipropyl- (9CI)
 MF C40 H53 F2 N3 O6 S

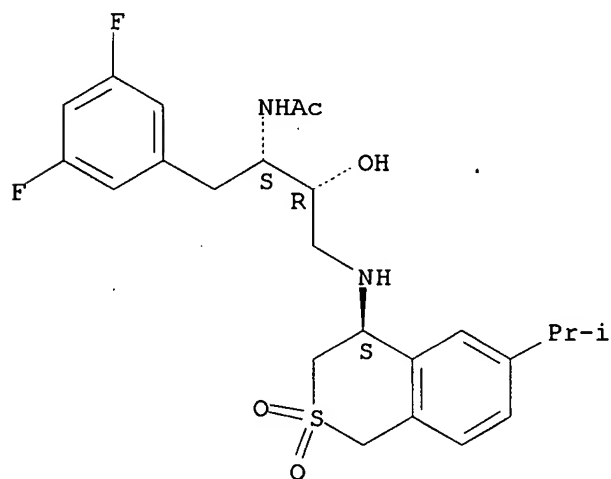
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[4S]-3,4-dihydro-6-(1-methylethyl)-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]- (9CI)
 MF C24 H30 F2 N2 O4 S

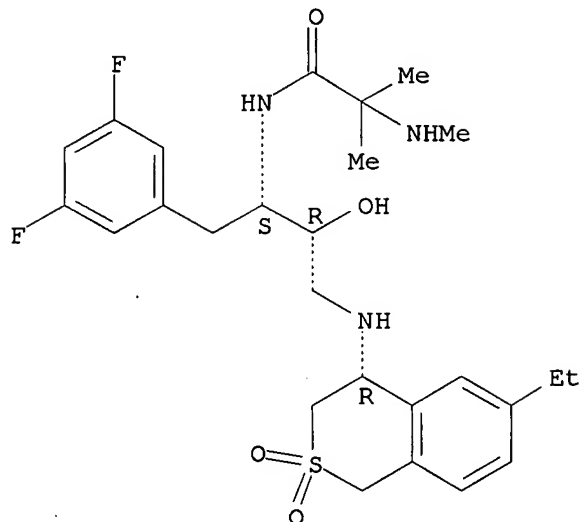
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[4R]-6-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-methyl-2-(methylethylamino)- (9CI)
 MF C26 H35 F2 N3 O4 S

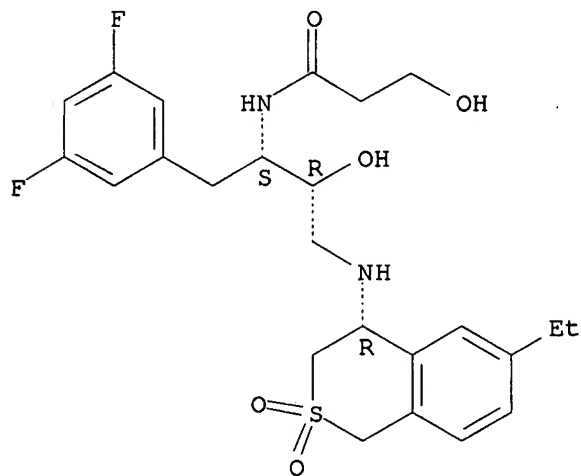
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[4-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-3-hydroxy- (9CI)
 MF C24 H30 F2 N2 O5 S

Absolute stereochemistry.

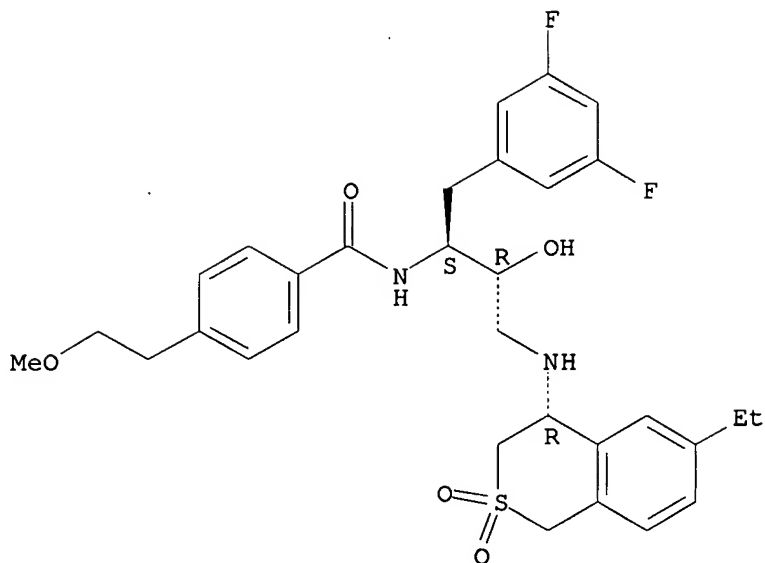


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
 IN Benzamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[4-ethyl-3,4-dihydro-2,2-dioxido-1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-4-(2-methoxyethyl)- (9CI)

MF C31 H36 F2 N2 O5 S

. Absolute stereochemistry.

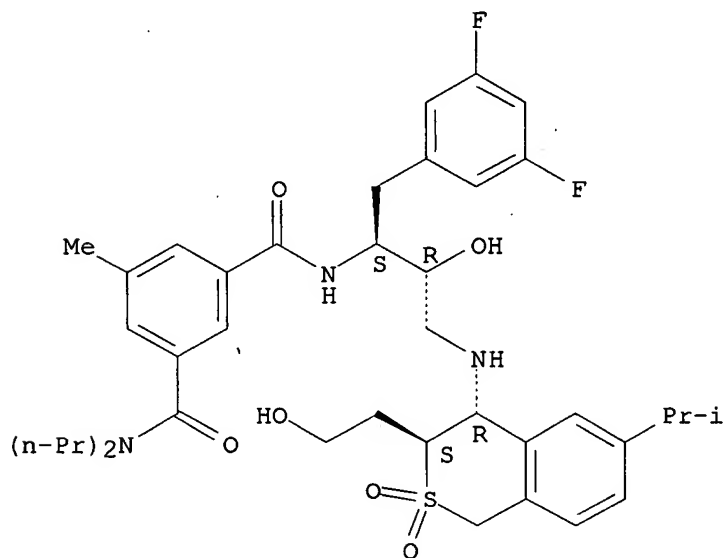


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 44 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-
3-[[[(3S,4R)-3,4-dihydro-3-(2-hydroxyethyl)-6-(1-methylethyl)-2,2-dioxido-
1H-2-benzothiopyran-4-yl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl-
(9CI)

MF C39 H51 F2 N3 O6 S

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT